

Paul Schulwitz please
Access DB# 103705

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SABIHA QA21 Examiner #: A4141 Date: 9/11/03
Art Unit: 1616 Phone Number 305-3910 Serial Number: 09/497,891
Mail Box and Bldg/Room Location: 2D19 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

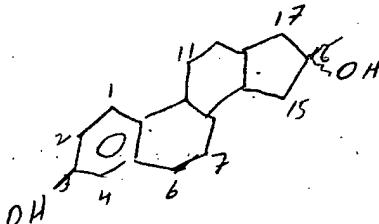
Title of Invention: 3,16-dihydroxy estra 1,3,5,(10) triene

Inventors (please provide full names): HERMAN KUENZER et al.

Earliest Priority Filing Date: 2/4/2000 DE 19906159

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for compds of formula in Cl 53
3,16 dihydroxy estra 1,3,5(10)-trien-
derivative



Please note, (1), no hydroxyl on 17-position
R¹⁷ may be a H, X, alkyl, sabs. or censubst.

(2) R⁷, X, H, alkyl, alkoxy.
You may leave other positions open?

Compds of Cl 64 can
be searched separately

Thank you.

STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: 9/12

Date Completed: 9/25/03

Searcher Prep & Review Time: 30

Clerical Prep Time: _____

Online Time: 27

Type of Search

NA Sequence (#) _____

Vendors and cost where applicable
STN 793.22

AA Sequence (#) _____

Dialog _____

Structure (#) 3

Questel/Orbit _____

Bibliographic _____

Dr.Link _____

Litigation _____

Lexis/Nexis _____

Fulltext _____

Sequence Systems _____

Patent Family _____

WWW/Internet _____

Other _____

Other (specify) _____

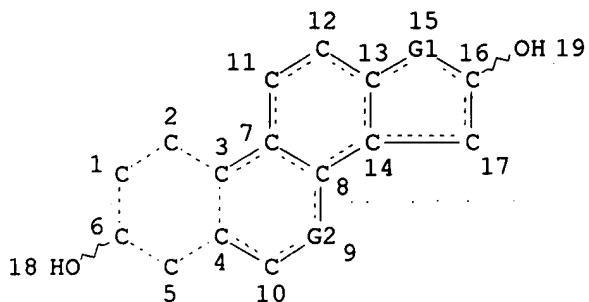
Claim 69

Qazi 09/497,891

September 25, 2003

=> d que
L1

STR



CH^vX
@20 21

CH^vAk
@22 23

CH^vX
@24 25

CH^vAk
@26 27 CH^vO^vAk
 @28 29 30

| 18 alpha-homo-estra-1,3,5(10)-triene -3,16 alpha-diol
not found

VAR G1=CH2/20/22

VAR G2=CH2/24/26/28

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DEFAULT ECLEVEL IS LIMITED

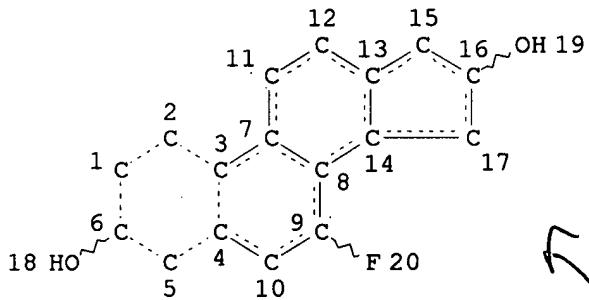
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L3 203 SEA FILE=REGISTRY SSS FUL L1
L13 STR



7 alpha fluoro

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

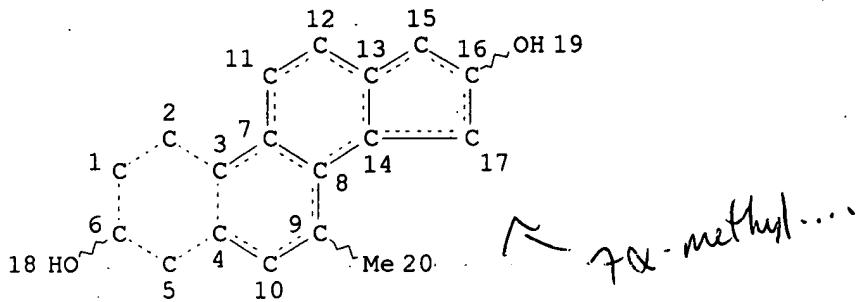
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RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L14 2 SEA FILE=REGISTRY SUB=L3 SSS FUL L13
L15 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L16 2 SEA FILE=REGISTRY SUB=L3 SSS FUL L15

L23 [REDACTED] 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14 OR L16

~~=> d 1b1b5 abs h1stcr~~

L23 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:552017 HCAPLUS

DOCUMENT NUMBER: 133:150782

TITLE: synthesis of 16-Hydroxyestratrienes as selectively effective estrogens

INVENTOR(S): Kuenzer, Hermann; Knauthe, Rudolf; Lessl, Monika; Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa; Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

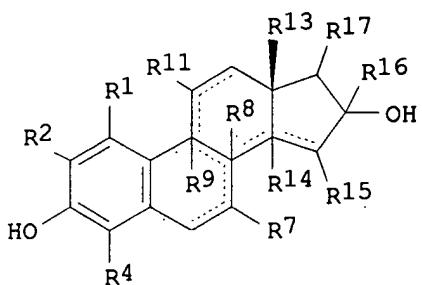
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,			

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2000029095	A5 20000829	AU 2000-29095	20000209
EP 1144431	A2 20011017	EP 2000-907539	20000209
EP 1144431	A3 20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
BR 2000008076	A 20020205	BR 2000-8076	20000209
JP 2002536455	T2 20021029	JP 2000-598520	20000209
EE 200100412	A 20021216	EE 2001-412	20000209
NO 2001003860	A 20011008	NO 2001-3860	20010808
BG 105804	A 20020329	BG 2001-105804	20010809
PRIORITY APPLN. INFO.:		DE 1999-19906159 A	19990209
		WO 2000-EP1073 W	20000209

OTHER SOURCE(S): MARPAT 133:150782
GI



AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2, CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16. α -estradiol shows a 50% uterine stimulation at 30 μ g in vivo testing.

IT 287721-57-7P 287721-58-8P 287721-71-5P

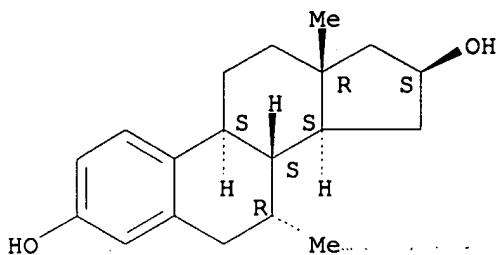
287721-85-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective estrogens)

RN 287721-57-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7. α .,16. β .)- (9CI)
(CA INDEX NAME)

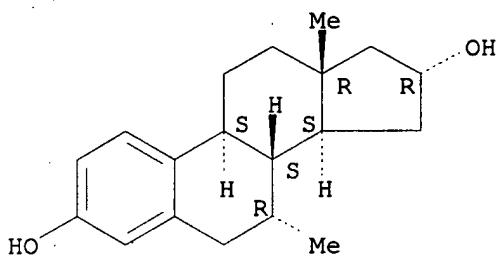
Absolute stereochemistry. Rotation (+).



RN 287721-58-8 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

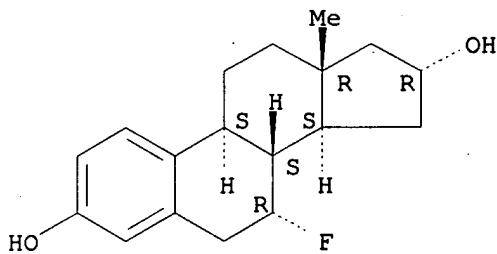
Absolute stereochemistry. Rotation (+).



RN 287721-71-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



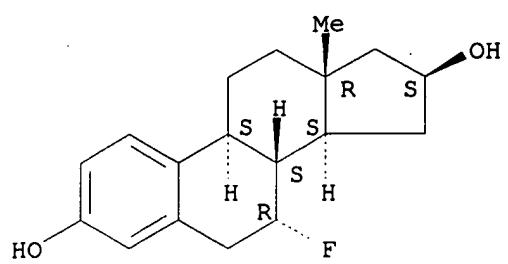
RN 287721-85-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

Qazi 09/497,891

September 25, 2003



Claim 53

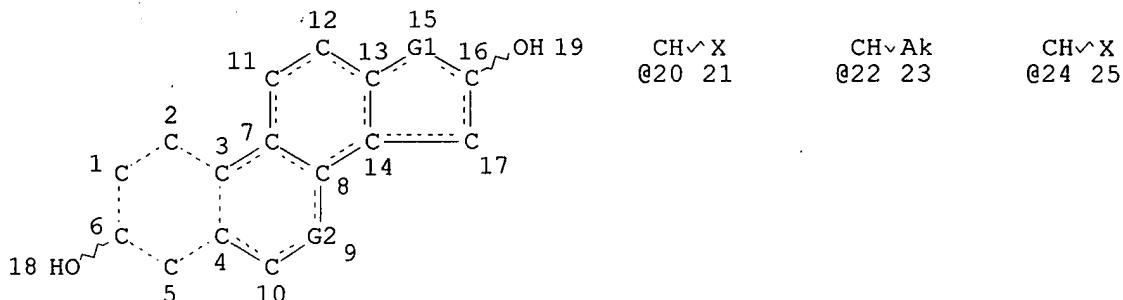
Qazi 09/497,891

September 25, 2003

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L1

STR



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CH^ O~Ak
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CH^ X
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CH^ Ak
@22 23

CH^ X
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VAR G1=CH2/20/22
VAR G2=CH2/24/26/28

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L3 203 SEA FILE=REGISTRY SSS FUL L1
L5 90 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

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L5 ANSWER 1 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:717656 HCAPLUS

DOCUMENT NUMBER: 138:50028

TITLE: Development and validation of an average mammalian estrogen receptor-based QSAR model

AUTHOR(S): Mekenyany, O.; Kamenska, V.; Serafimova, R.; Poellinger, L.; Brouwer, A.; Walker, J.

CORPORATE SOURCE: Laboratory of Mathematical Chemistry, University "As. Zlatarov", Bourgas, 8010, Bulg.

SOURCE: SAR and QSAR in Environmental Research (2002), 13(6), 579-595

PUBLISHER: CODEN: SQERED; ISSN: 1062-936X

DOCUMENT TYPE: Taylor & Francis Ltd.

LANGUAGE: English

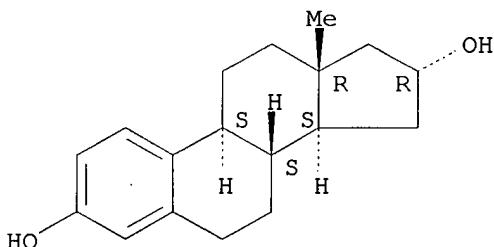
AB Development and evaluation of quant. structure activity relationships (QSARs) for predicting estrogen receptor binding from chem. structure requires reliable algorithms for three-dimensional (3D) QSAR anal. and establishment of structurally diverse training sets of chems. whose modes of action and measures of potency are well defined. One approach to

Selecting an appropriate training set is to minimize the biol. variability in the model development, by using structurally restricted data sets. A second approach is to extend the structural diversity of chems. at the cost of increased variability of biol. assays. In this study, the second approach was used by organizing a training set of 151 chems. with measured human alpha Estrogen Receptor (ER.alpha.), mouse uterine, rat uterine, and MCF7 cell Relative Binding Affinities (RBAs). The structurally augmented training set was submitted to a 3D pattern recognition anal. to derive a model for av. mammalian ER binding affinity by employing the CCommon REactivity PAttern (COREPA) approach. Elucidation of this pattern required examn. of the conformational flexibility of the compds. to reveal areas in the multidimensional descriptor space, which are most populated by the conformers of the biol. active mols. and least populated by the inactive ones. The approach is not dependent upon a predetd. and specified toxicophore or an alignment of conformers to a lead compd. Reactivity patterns assocd. with mammalian ER binding affinity were obtained in terms of global nucleophilicity (EHOMO), interat. distances between nucleophilic sites, and local nucleophilicity (charges or delocalizabilities) of those sites. Based on derived patterns, descriptor profiles were established for identifying and ranking compds. with RBA of >150, 150-10, 10-1 and 1-0.1% relative to 17.beta.-estradiol. Specificity of reactivity profiles was found to increase gradually with increasing affinities assocd. with RBAs ranges under study. Using the results of this anal., an exploratory expert system was developed for use in ranking relative mammalian ER binding affinity potential for large chem. data sets. The validity of the RBA predictions were confirmed by independent development and comparison with measured RBA values.

IT 1090-04-6, 16.alpha.-Estradiol
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (development and validation of an av. mammalian estrogen receptor-based QSAR model)

RN 1090-04-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:122822 HCAPLUS
 DOCUMENT NUMBER: 136:161698
 TITLE: Combination preparation with an ER.beta. selective estrogen and a SERM or antiestrogen
 INVENTOR(S): Fritzemeier, Karl-Heinrich; Kollenkirchen, Uwe;

PATENT ASSIGNEE(S): Hegele-Hartung, Christa
 SOURCE: Schering Aktiengesellschaft, Germany
 PCT Int. Appl., 33 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

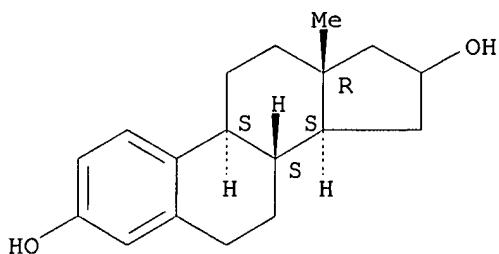
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002011765	A1	20020214	WO 2001-EP9008	20010803
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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DE 10039199	A1	20020221	DE 2000-10039199	20000810
AU 2001093720	A5	20020218	AU 2001-93720	20010803
EP 1307229	A1	20030507	EP 2001-974107	20010803
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRIORITY APPLN. INFO.:			DE 2000-10039199 A	20000810
			WO 2001-EP9008	W 20010803

AB A novel medicament for the treatment of estrogen-deficient disease states is disclosed. Said medicament is a combination prepn. comprising an ER.beta.-selective estrogen and an ER.alpha.-selective antiestrogen or SERM (Selective Estrogen Receptor Modulator). The antiestrogen or SERM which is a component of the combination prepn. is preferably selective for the periphery. The prepn. is suitable for an organ-specific estrogen therapy and has clear advantages over conventional therapies. Due to the combination of ER.alpha.-selective SERM and ER.beta.-estrogen the prepn. permits a complete protection against bone loss caused by estrogen deficiency. The components of the medicament also have a synergistic effect with respect to the inhibition of inflammation inducing genes, in particular in inflammatory disorders such as atherosclerosis and arthritis, or neurodegenerative diseases such as Alzheimers and multiple sclerosis. Furthermore, pos. effects on cognition and mood may be expected. The protective estrogen-like effects are achieved, with no expectation of proliferation effects on breasts or uterus.

IT 397872-24-1D, Estra-1,3,5(10)-triene-3,16-diol, derivs.
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (combination prepn. with an ER.beta. selective estrogen and a SERM or antiestrogen)

RN 397872-24-1 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:190285 HCPLUS

DOCUMENT NUMBER: 134:261332

TITLE: QSAR with electrotopological state atom index.

Part-3a. Receptor binding affinity of estrogens and non-steroidal estrogen analogs

AUTHOR(S): Saha, Achintya; Roy, Kunal; De, Kakali; Sengupta, Chandana

CORPORATE SOURCE: Dep. Chemical Technology, Univ. Calcutta, alcutta, 700 009, India

SOURCE: Journal of the Indian Chemical Society (2001), 78(2), 92-97

CODEN: JICSAH; ISSN: 0019-4522

PUBLISHER: Indian Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Quant. structure activity relationship (QSAR) anal. of estrogens and non-steroidal analogs of estrogen with electrotopol. state atom (ETSA) index has been performed to explore the atoms or fragments of the mols. that are most important for the binding affinity to receptor. The study reveals the importance of Ph ring fragment (C1, C5 and C10 atoms of steroid estrogen, and C1, C3, C4, C9 and C10 atoms in case of non-steroidal analogs) for receptor binding affinity. The importance of these atoms or fragments is also supported from the literature survey. Thus, the Ph ring constitutes the pharmacophore for receptor binding affinity of estrogen analogs. Hence, diagnostic potential of the ETSA scheme in identifying the atoms or fragments important for activity is revealed from the study.

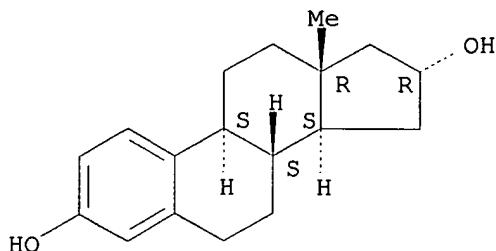
IT 1090-04-6

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(QSAR with electrotopol. state atom index in relation to receptor binding affinity of estrogens and non-steroidal estrogen analogs)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:898420 HCPLUS

DOCUMENT NUMBER: 134:80974

TITLE: A computationally based identification algorithm for estrogen receptor ligands: Part 2. Evaluation of a hER. α . binding affinity model

AUTHOR(S): Mekenyanyan, O. G.; Kamenska, V.; Schmieder, P. K.; Ankley, G. T.; Bradbury, S. P.

CORPORATE SOURCE: Laboratory of Mathematical Chemistry, Department of Physical Chemistry, Bourgas University "Prof. As. Zlataarov.", Bourgas, 118010, Bulg.

SOURCE: Toxicological Sciences (2000), 58(2), 270-281
CODEN: TOSCF2; ISSN: 1096-6080

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The objective of this study was to evaluate the capability of an expert system described in the previous paper to identify the potential for chems. to act as ligands of mammalian estrogen receptors (ERs). The basis of the expert system was a structure activity relationship (SAR) model, based on relative binding affinity (RBA) values for steroid and nonsteroidal chems. derived from human ER. α . (hER. α .) competitive binding assays. The expert system enables categorization of chems. into RBA ranges of <0.1, 0.1 to 1, 1 to 10, 10 to 100, and >150% relative to 17. β -estradiol. In the current anal., the algorithm was evaluated with respect to predicting RBAs of chems. assayed with ERs from MCF7 cells, and mouse and rat uterine preps. The best correspondence between predicted and obsd. RBA ranges was obtained with MCF7 cells. The agreement between predictions from the expert system and data from binding assays with mouse and rat ER(s) were less reliable, esp. for chems. with RBAs less than 10%. Prediction errors often were false positives, i.e., predictions of greater than obsd. RBA values. While discrepancies were likely due, in part, to species-specific variations in ER structure and ligand binding affinity, a systematic bias in structural characteristics of chems. in the hER. α . training set, compared to the rodent evaluation data sets, also contributed to prediction errors. False-pos. predictions were typically assocd. with ligands that had shielded electroneg. sites. Ligands with these structural characteristics were not well represented in the training set used to derive the expert system. Inclusion of a shielding criterion into the original expert system significantly increased the accuracy of RBA predictions. With this addnl. structural requirement, 38 of 46 compds. with measured RBA values greater than 10% in hER. α ., MCF7, and rodent uterine preps. were correctly

categorized. Of the remaining 129 compds. in the combined data sets, RBA values for 65 compds. were correctly predicted, with 47 of the incorrect predictions being false positives. Based upon this exploratory anal., the modeling approach, combined with a high-quality training set of RBA values derived from a diverse set of chem. structures, could provide a credible tool for prioritizing chems. with moderate to high ER binding affinity for subsequent in vitro or in vivo assessments.

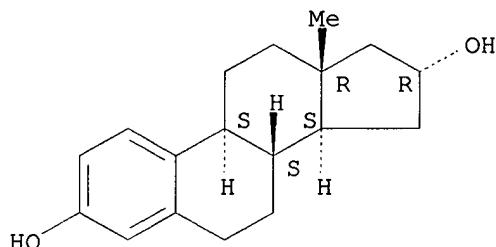
IT 1090-04-6, 16.alpha.-Estradiol

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(computationally based identification algorithm for estrogen receptor ligand .alpha. binding affinity)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:738805 HCAPLUS

DOCUMENT NUMBER: 133:296594

TITLE: Preparation of ent-steroids as selectively effective estrogens

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19917930	A1	20001019	DE 1999-19917930	19990415
WO 2000063228	A1	20001026	WO 2000-EP3470	20000417
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
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EP 1169336 A1 20020109 EP 2000-925219 20000417
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 IE, SI, LT, LV, FI, RO
 JP 2002542255 T2 20021210 JP 2000-612318 20000417
 PRIORITY APPLN. INFO.: DE 1999-19917930 A 19990415
 WO 2000-EP3470 W 20000417

OTHER SOURCE(S): MARPAT 133:296594

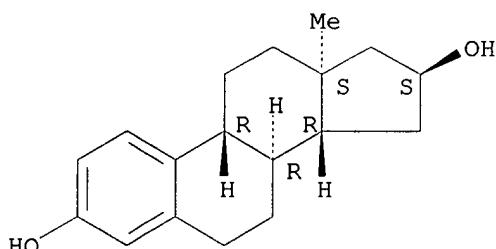
AB The invention describes new ent-steroids I [R1 = H, OR12, alkenyloxy, alkynyoxy, OSO2R13; R2 = OR12, OSO2R13, OC(:O)R16; R3, R4, R5, R8, R9 = H, halogen, OR12, OSO2R13, R16; R6 = .beta.-H; R7 = H; R6R7 = .alpha.-, .beta.-CH2; R10 = H2, dihalogen, H and a halogen, :CR17R18; R11 = H, Me, Et; R12 = H, C1-5-alkyl, C1-5-alkenyl; R13 = , NR14R15; R14, R15 = H, C1-5-alkyl, COR16, C3-7-cycloalky, aryl; R14R15 = polymethylene; NR14R15 = morpholine; R16 = C1-12-alkyl, C1-12-alkenyl, C1-12-alkynyl; R17, R18 = H, halogen, H and OR12, H and OSO2R13, R12 and OC(:O)R16, O; one or more double bonds at C(6)-C(7), C(7)-C(8), C(8)-C(9), C(9)-C(11), C(11)-C(12), C(8)-C(14), C(14)-C(15), C(15)-C(16), C(16)-C(17)], as pharmaceutically active substances, which exhibit in vitro a higher affinity at estrogen receptor of rat prostate than at estrogen receptor of Rat uterus and in vivo a preferential effect at the bone in the comparison to the uterus, their prodn., its therapeutic application and pharmaceutical compns., which contain the new compds. Thus, ent-estriol (I; R1 = R3 = R4 = R5 = R6 = R7 = R8 = H, R2 = OH, R9 = .alpha.-OH, R10 = .beta.-OH, R11 = Me) was prep'd. stereoselectively from ent-3,16.alpha.-dihydroxyestra-1,3,5(10)-trien-17-one (I; R1 = R3 = R4 = R5 = R6 = R7 = R8 = H, R2 = OH, R9 = .alpha.-OH, R10 = O, R11 = Me) via redn. with NaBH4 in MeOH. Furthermore the invention describes the use of steroids, those with the (8.alpha.-H,9.beta.-H,10.alpha.-H,13.alpha.-H,14.beta.-H)-gonane skeleton, for the treatment of estrogen deficiency conditioned diseases and conditions.

IT 300853-08-1P, ent-Estra-1,3,5(10)-triene-3,16.alpha.-diol
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prep'n. of ent-steroids as selectively effective estrogens)

RN 300853-08-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (8.alpha.,9.beta.,13.alpha.,14.beta.,16.
 beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:552017 HCAPLUS

DOCUMENT NUMBER: 133:150782

TITLE: synthesis of 16-Hydroxyestratrienes as selectively

effective estrogens

INVENTOR(S): Kuenzer, Hermann; Knauthe, Rudolf; Lessl, Monika;
 Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa;
 Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 2000029095	A5	20000829	AU 2000-29095	20000209
EP 1144431	A2	20011017	EP 2000-907539	20000209
EP 1144431	A3	20020612		
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BR 2000008076	A	20020205	BR 2000-8076	20000209
JP 2002536455	T2	20021029	JP 2000-598520	20000209
EE 200100412	A	20021216	EE 2001-412	20000209
NO 2001003860	A	20011008	NO 2001-3860	20010808
BG 105804	A	20020329	BG 2001-105804	20010809
PRIORITY APPLN. INFO.:			DE 1999-19906159 A	19990209
			WO 2000-EP1073 W	20000209

OTHER SOURCE(S): MARPAT 133:150782

AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2, CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16.alpha.-estradiol shows a 50% uterine stimulation at 30 .upsilon.g in in vivo testing.

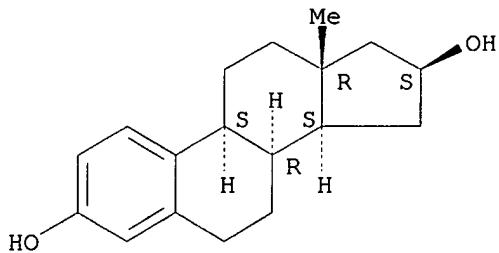
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287722-16-1P 287722-17-2P 287722-18-3P
287722-19-4P 287722-20-7P 287722-22-9P
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287723-22-2P 287724-23-6P 287724-24-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective estrogens)

RN 287721-55-5 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (8.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

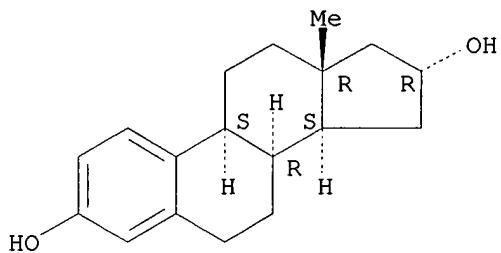
Absolute stereochemistry. Rotation (+).



RN 287721-56-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (8.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

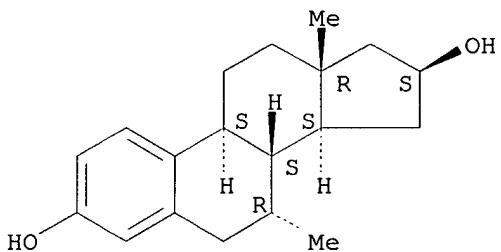
Absolute stereochemistry. Rotation (+).



RN 287721-57-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

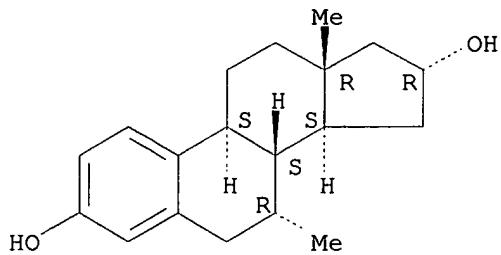
Absolute stereochemistry. Rotation (+).



RN 287721-58-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

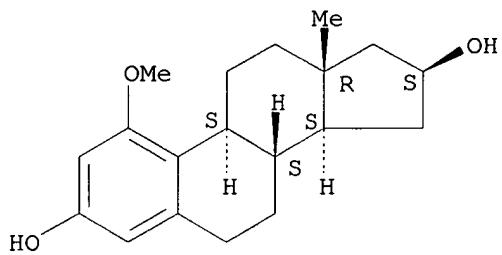
Absolute stereochemistry. Rotation (+).



RN 287721-59-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16.beta.)- (9CI) (CA INDEX NAME)

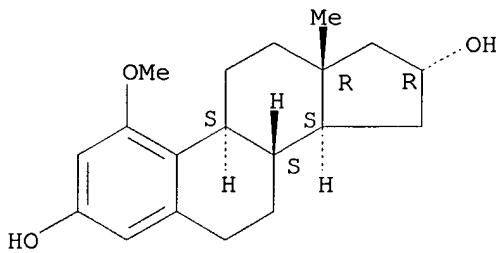
Absolute stereochemistry.



RN 287721-60-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16.alpha.)- (9CI) (CA INDEX NAME)

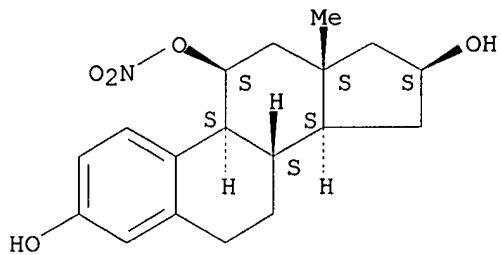
Absolute stereochemistry.



RN 287721-61-3 HCPLUS

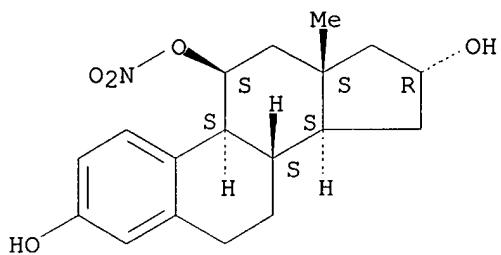
CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate, (11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



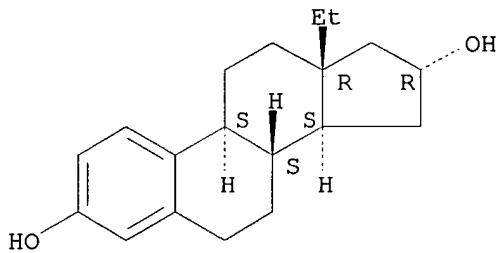
RN 287721-62-4 HCPLUS
 CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate, (11.beta.,16.alpha.)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



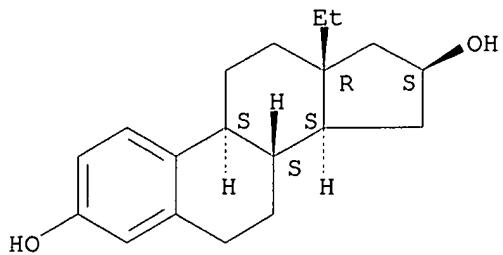
RN 287721-63-5 HCPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16.alpha.)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



RN 287721-64-6 HCPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16.beta.)- (9CI) (CA INDEX
 NAME)

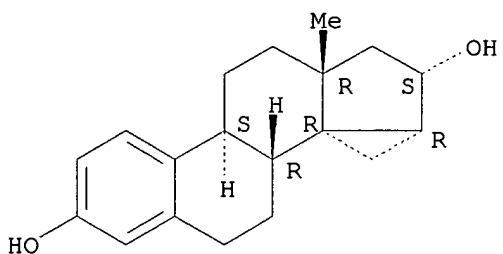
Absolute stereochemistry. Rotation (+).



RN 287721-66-8 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14R,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

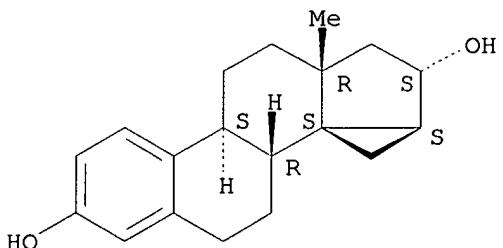
Absolute stereochemistry.



RN 287721-67-9 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14S,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

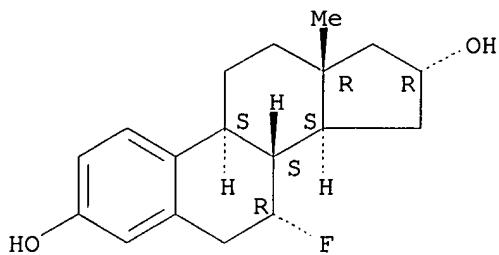
Absolute stereochemistry.



RN 287721-71-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

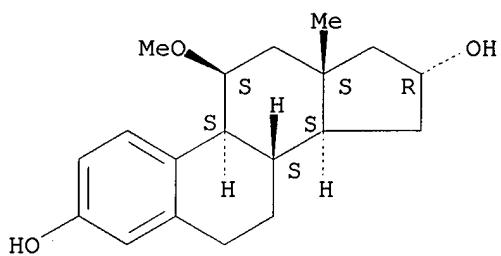
Absolute stereochemistry.



RN 287721-72-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-, (11.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

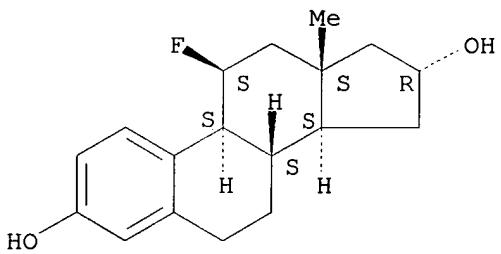
Absolute stereochemistry.



RN 287721-73-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

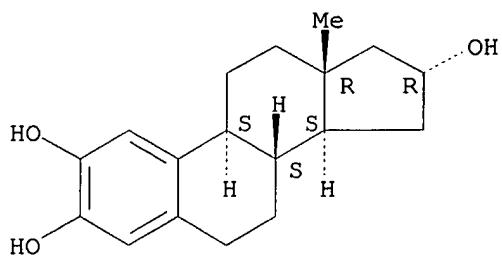
Absolute stereochemistry.



RN 287721-74-8 HCPLUS

CN Estra-1,3,5(10)-triene-2,3,16-triol, (16.alpha.)- (9CI) (CA INDEX NAME)

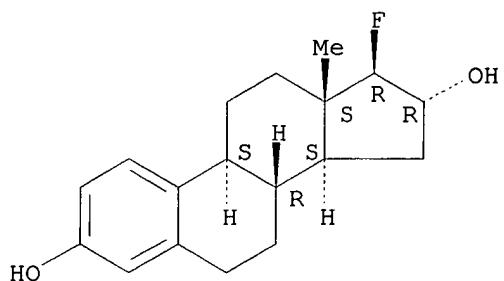
Absolute stereochemistry.



RN 287721-75-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16.alpha.,17.beta.)- (9CI)
(CA INDEX NAME)

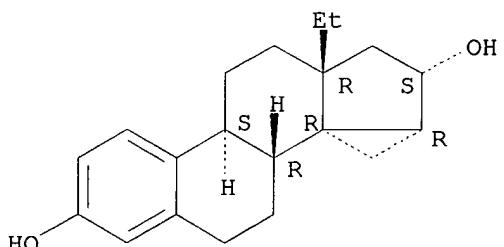
Absolute stereochemistry.



RN 287721-77-1 HCPLUS

CN Cyclopropano[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-,
(14R,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

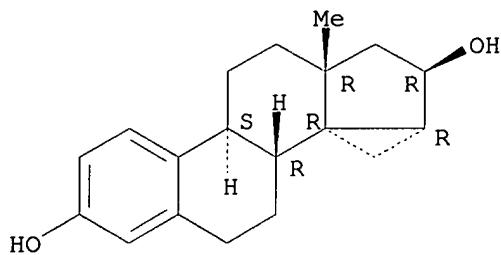
Absolute stereochemistry.



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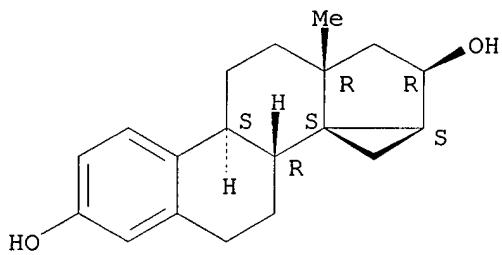
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14R,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



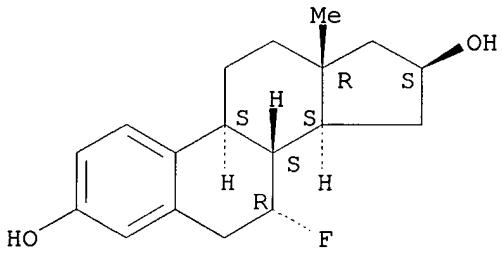
RN 287721-81-7 HCAPLUS
 CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
 (14S,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



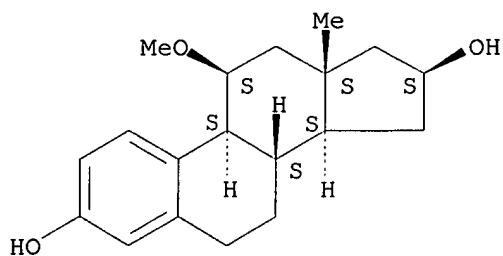
RN 287721-85-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.beta.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-86-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-, (11.beta.,16.beta.)- (9CI)
 (CA INDEX NAME)

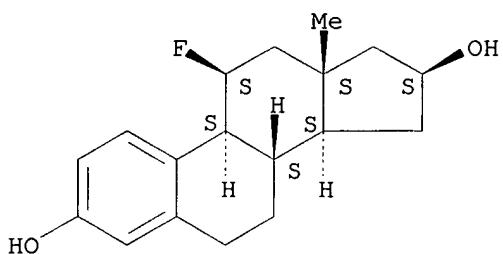
Absolute stereochemistry.



RN 287721-87-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

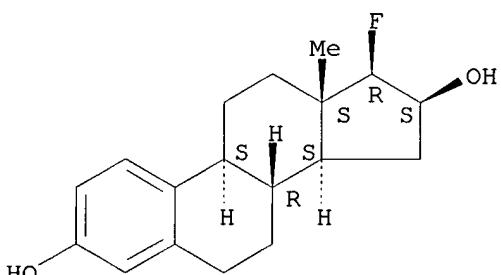
Absolute stereochemistry.



RN 287721-88-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16.beta.,17.beta.)- (9CI)
(CA INDEX NAME)

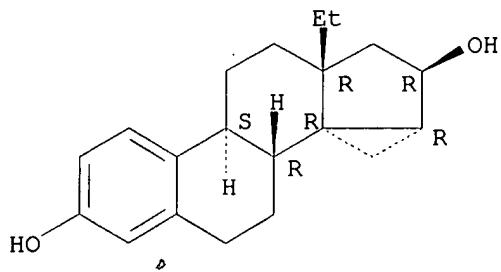
Absolute stereochemistry.



RN 287721-90-8 HCAPLUS

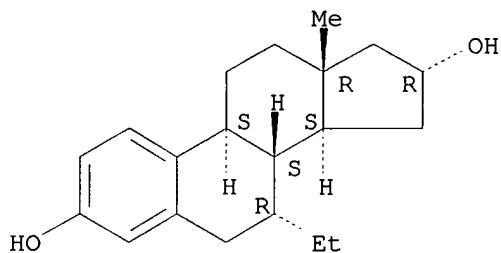
CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-,
(14R,15beta.,16beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



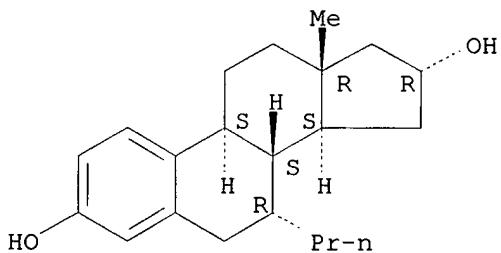
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 (CA INDEX NAME)

Absolute stereochemistry.



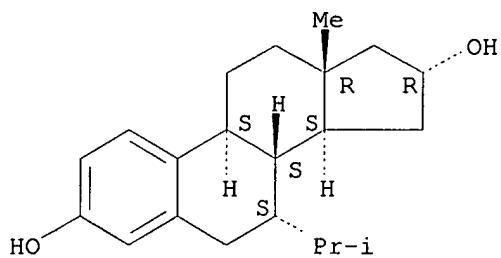
RN 287721-94-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7.alpha.,16.alpha.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-95-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.alpha.,16.alpha.)-
 (9CI) (CA INDEX NAME)

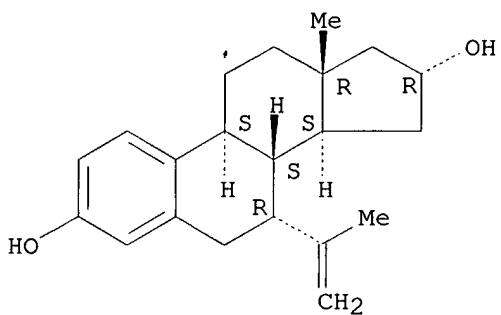
Absolute stereochemistry.



RN 287721-96-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

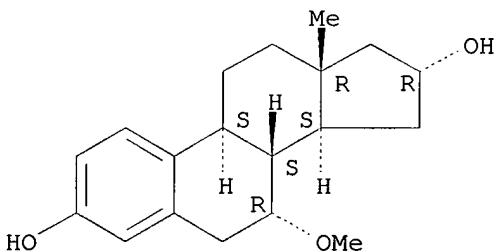
Absolute stereochemistry.



RN 287721-98-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

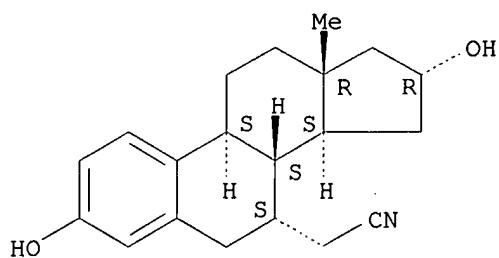
Absolute stereochemistry.



RN 287722-00-3 HCPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

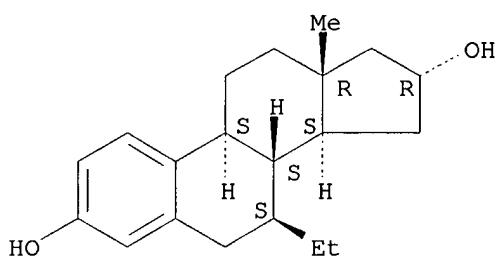
Absolute stereochemistry.



RN 287722-01-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

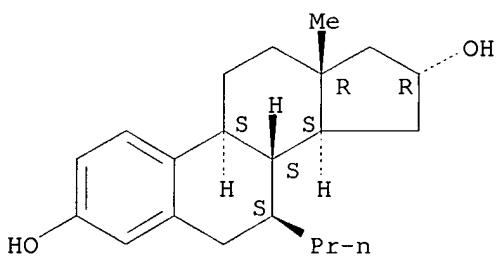
Absolute stereochemistry.



RN 287722-02-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

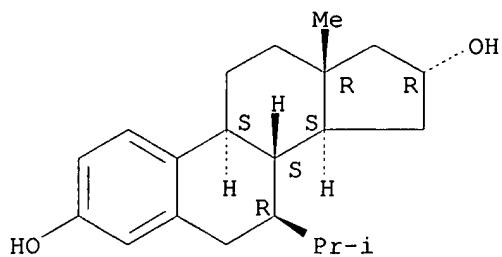
Absolute stereochemistry.



RN 287722-03-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.beta.,16.alpha.)-
(9CI) (CA INDEX NAME)

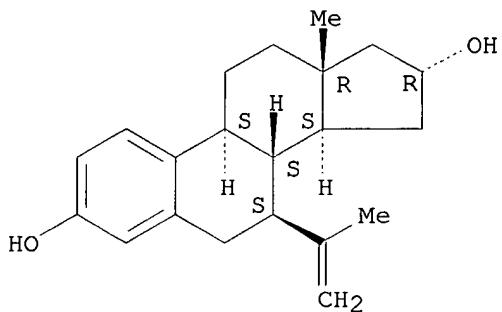
Absolute stereochemistry.



RN 287722-04-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

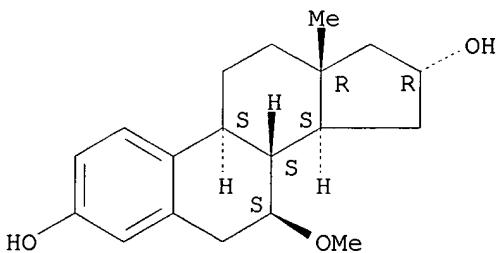
Absolute stereochemistry.



RN 287722-06-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

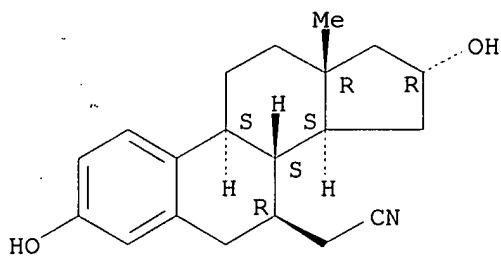
Absolute stereochemistry.



RN 287722-08-1 HCPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

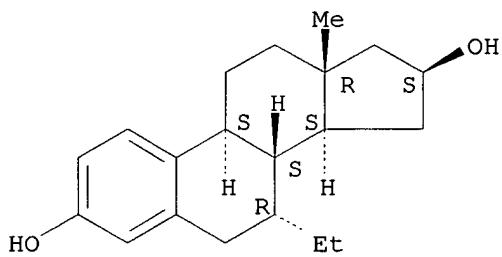
Absolute stereochemistry.



RN 287722-09-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7. α .,16. β .)- (9CI)
(CA INDEX NAME)

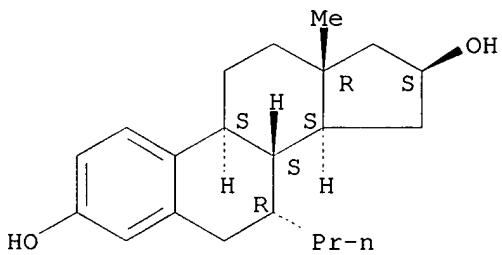
Absolute stereochemistry.



RN 287722-10-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7. α .,16. β .)- (9CI)
(CA INDEX NAME)

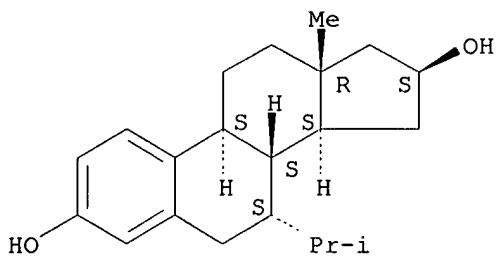
Absolute stereochemistry.



RN 287722-11-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7. α .,16. β .)-
(9CI) (CA INDEX NAME)

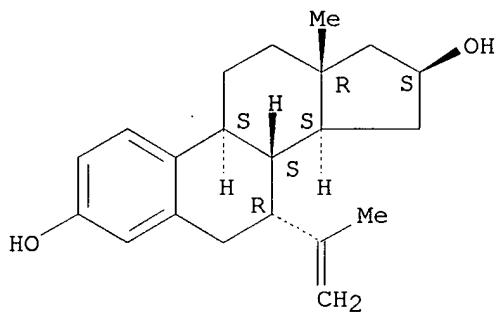
Absolute stereochemistry.



RN 287722-12-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
 (7. α .,16. β .)- (9CI) (CA INDEX NAME)

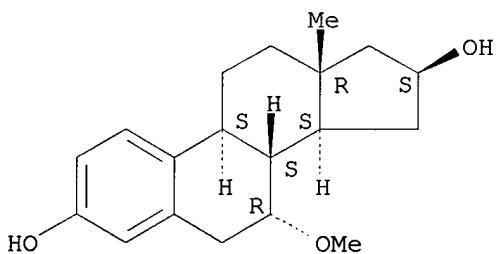
Absolute stereochemistry.



RN 287722-14-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7. α .,16. β .)- (9CI)
 (CA INDEX NAME)

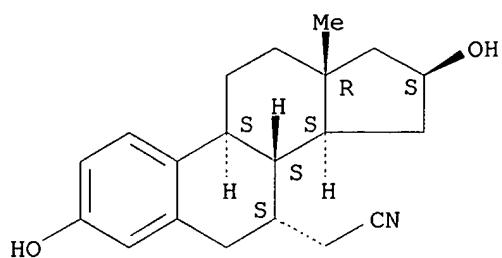
Absolute stereochemistry.



RN 287722-16-1 HCPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
 (7. α .,16. β .)- (9CI) (CA INDEX NAME)

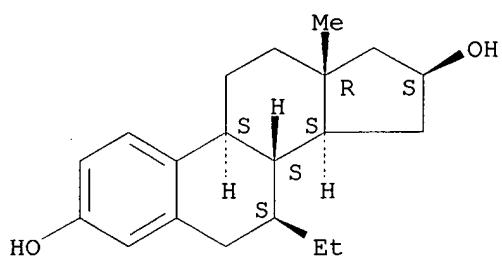
Absolute stereochemistry.



RN 287722-17-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

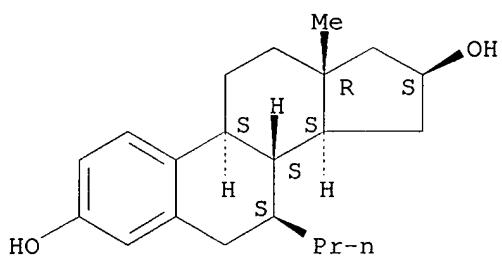
Absolute stereochemistry.



RN 287722-18-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

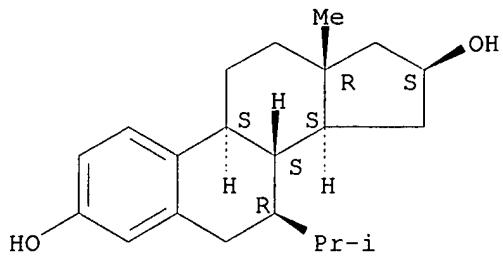
Absolute stereochemistry.



RN 287722-19-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

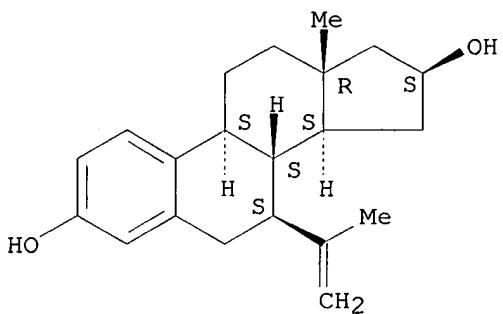
Absolute stereochemistry.



RN 287722-20-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

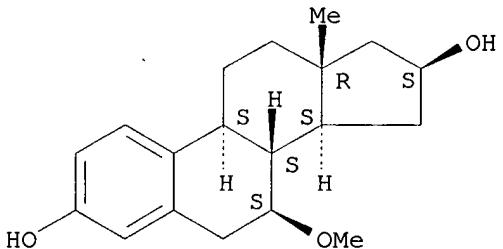
Absolute stereochemistry.



RN 287722-22-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

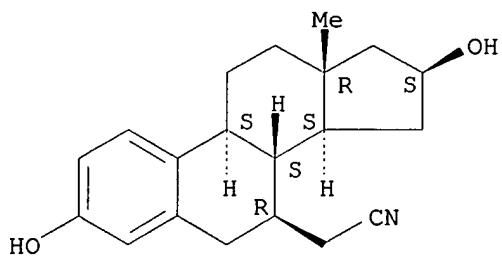
Absolute stereochemistry.



RN 287722-24-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

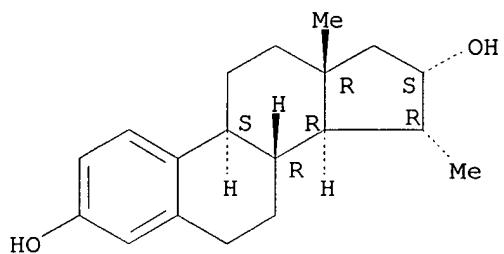
Absolute stereochemistry.



RN 287722-25-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15. α ,16. α)-(9CI)
(CA INDEX NAME)

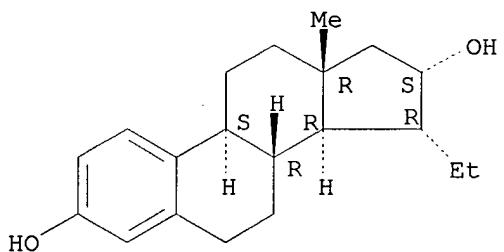
Absolute stereochemistry.



RN 287722-26-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15. α ,16. α)-(9CI)
(CA INDEX NAME)

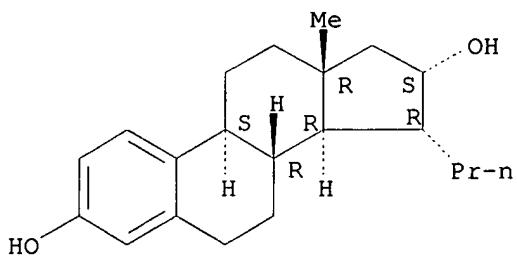
Absolute stereochemistry.



RN 287722-27-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15. α ,16. α)-(9CI)
(CA INDEX NAME)

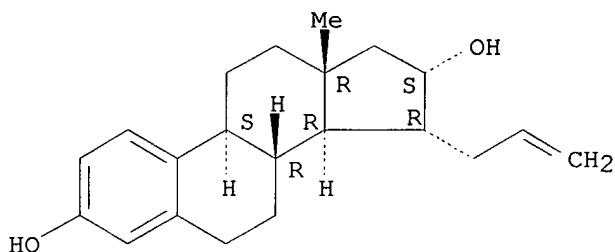
Absolute stereochemistry.



RN 287722-28-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15. α ,16. α .)-
(9CI) (CA INDEX NAME)

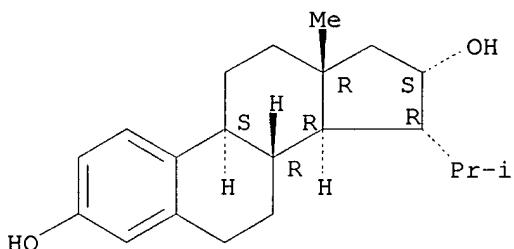
Absolute stereochemistry.



RN 287722-29-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15. α ,16. α .)- (9CI) (CA INDEX NAME)

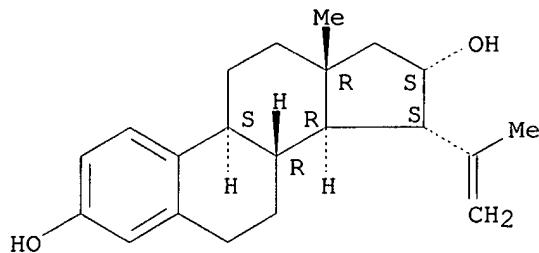
Absolute stereochemistry.



RN 287722-30-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15. α ,16. α .)- (9CI) (CA INDEX NAME)

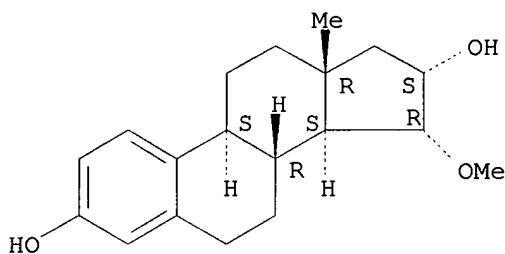
Absolute stereochemistry.



RN 287722-31-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15. α ,16. α)-(9CI) (CA INDEX NAME)

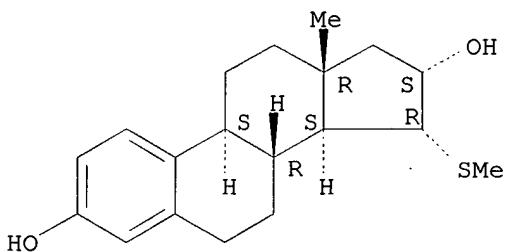
Absolute stereochemistry.



RN 287722-32-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15. α ,16. α)-(9CI) (CA INDEX NAME)

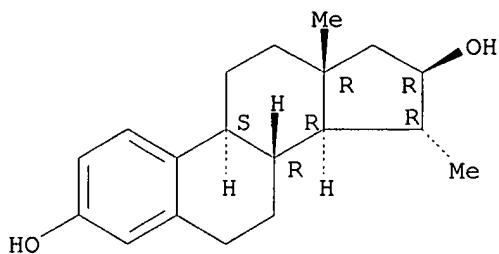
Absolute stereochemistry.



RN 287722-33-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15. α ,16. β)-(9CI) (CA INDEX NAME)

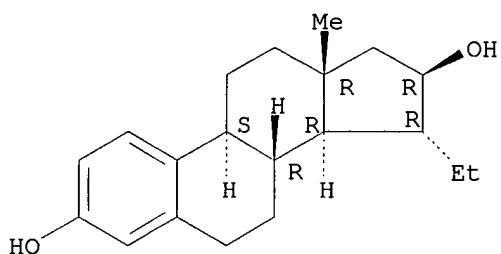
Absolute stereochemistry.



RN 287722-34-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

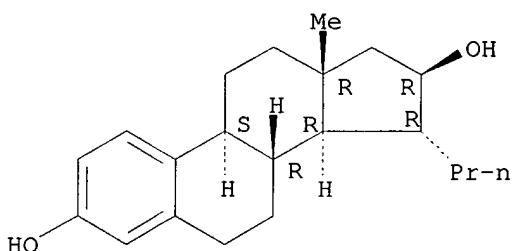
Absolute stereochemistry.



RN 287722-35-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

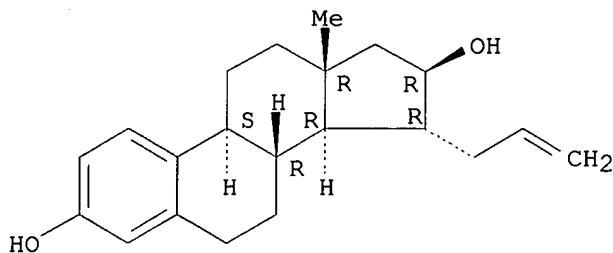
Absolute stereochemistry.



RN 287722-36-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15.alpha.,16.beta.)-
(9CI) (CA INDEX NAME)

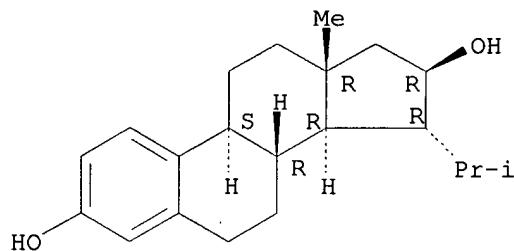
Absolute stereochemistry.



RN 287722-37-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15.α.,16.β.)- (9CI) (CA INDEX NAME)

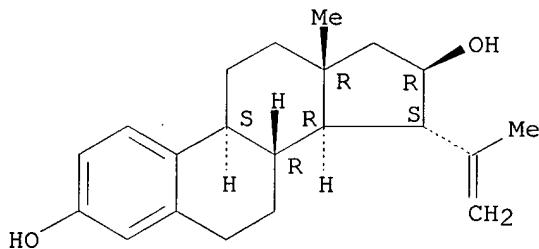
Absolute stereochemistry.



RN 287722-38-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15.α.,16.β.)- (9CI) (CA INDEX NAME)

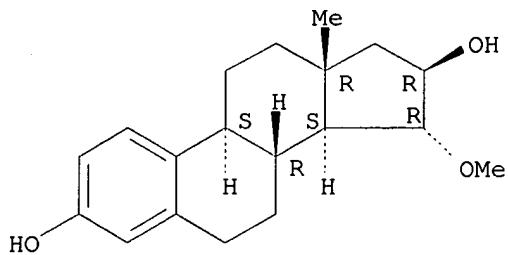
Absolute stereochemistry.



RN 287722-39-8 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15.α.,16.β.)- (9CI)
(CA INDEX NAME)

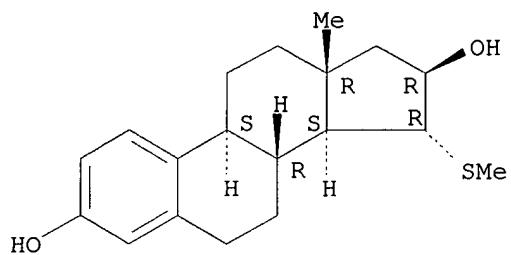
Absolute stereochemistry.



RN 287722-40-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15.alpha.,16.beta.)-
(9CI) (CA INDEX NAME)

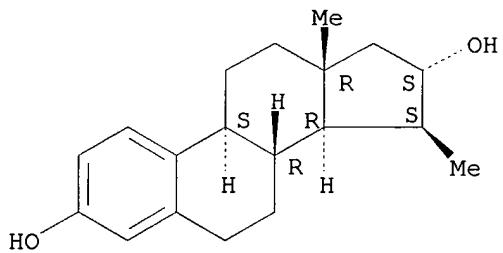
Absolute stereochemistry.



RN 287722-41-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

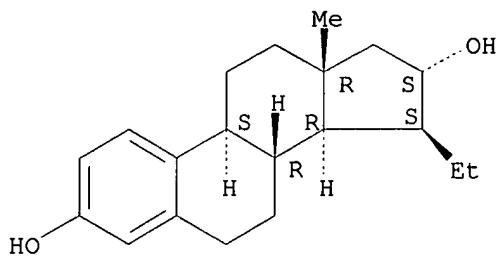
Absolute stereochemistry.



RN 287722-42-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

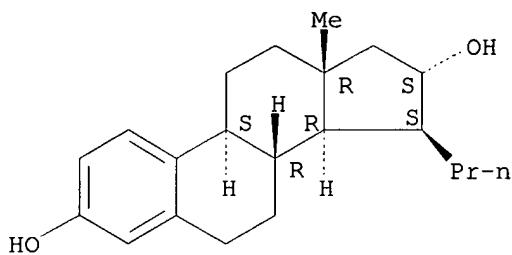
Absolute stereochemistry.



RN 287722-43-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15. β .,16. α .)- (9CI) (CA INDEX NAME)

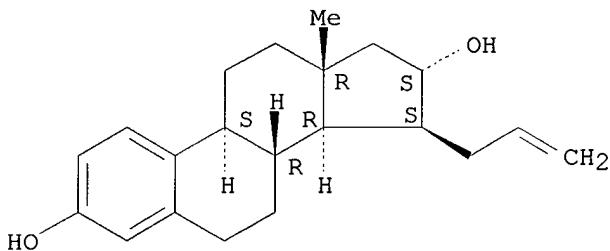
Absolute stereochemistry.



RN 287722-44-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15. β .,16. α .)- (9CI) (CA INDEX NAME)

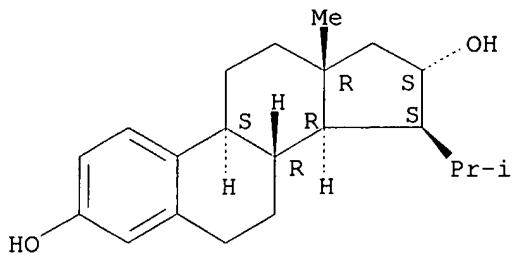
Absolute stereochemistry.



RN 287722-45-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-, (15. β .,16. α .)- (9CI) (CA INDEX NAME)

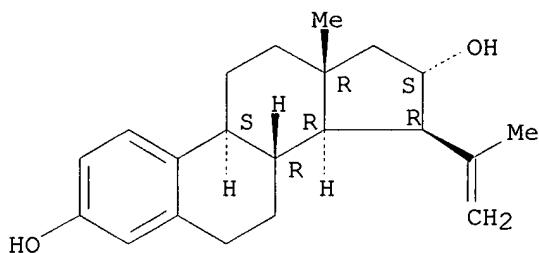
Absolute stereochemistry.



RN 287722-46-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15.β.,16.α.)- (9CI) (CA INDEX NAME)

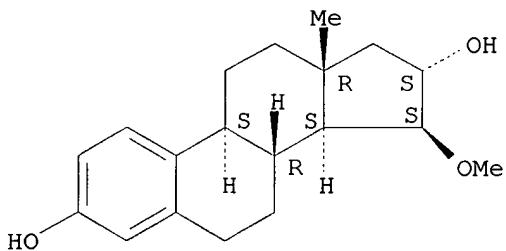
Absolute stereochemistry.



RN 287722-47-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15.β.,16.α.)- (9CI)
(CA INDEX NAME)

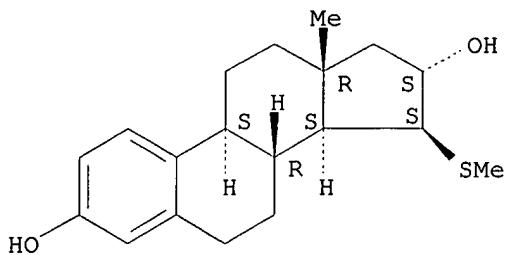
Absolute stereochemistry.



RN 287722-48-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15.β.,16.α.)-
(9CI) (CA INDEX NAME)

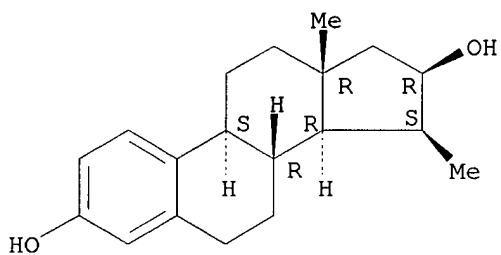
Absolute stereochemistry.



RN 287722-49-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15. β .,16. β .)- (9CI)
(CA INDEX NAME)

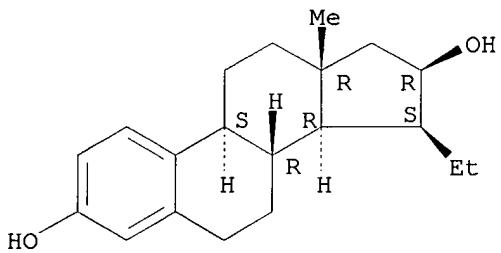
Absolute stereochemistry.



RN 287722-50-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15. β .,16. β .)- (9CI)
(CA INDEX NAME)

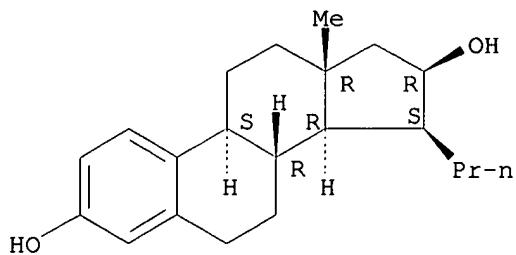
Absolute stereochemistry.



RN 287722-51-4 HCPLUS

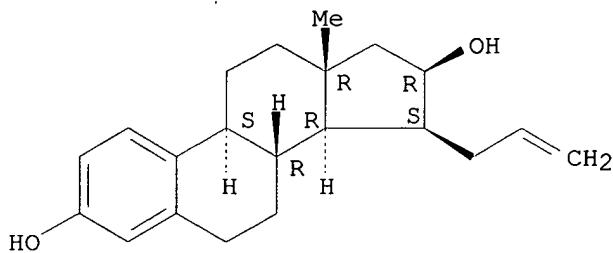
CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15. β .,16. β .)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



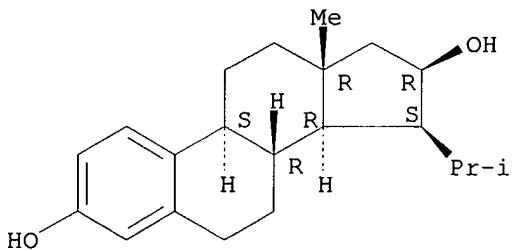
RN 287722-52-5 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15. β .,16. β .)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



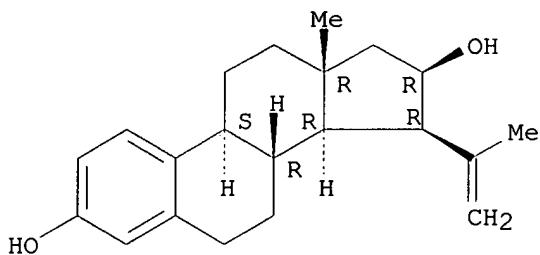
RN 287722-53-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
 (15. β .,16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-54-7 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
 (15. β .,16. β .)- (9CI) (CA INDEX NAME)

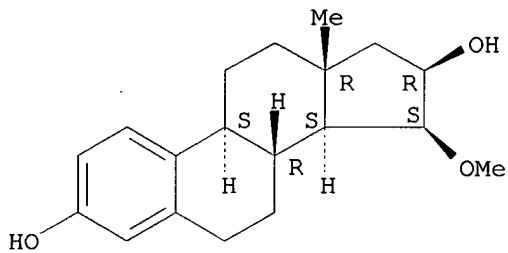
Absolute stereochemistry.



RN 287722-55-8 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15. β .,16. β .)- (9CI)
(CA INDEX NAME)

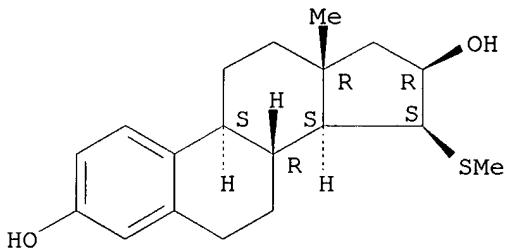
Absolute stereochemistry.



RN 287722-56-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15. β .,16. β .)-
(9CI) (CA INDEX NAME)

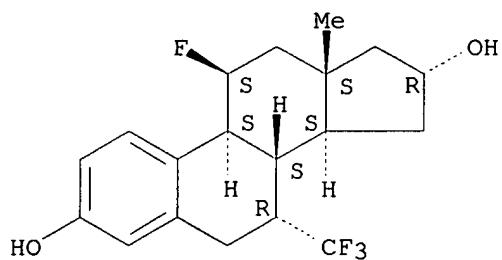
Absolute stereochemistry.



RN 287722-57-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(trifluoromethyl)-,
(7. α .,11. β .,16. α .)- (9CI) (CA INDEX NAME)

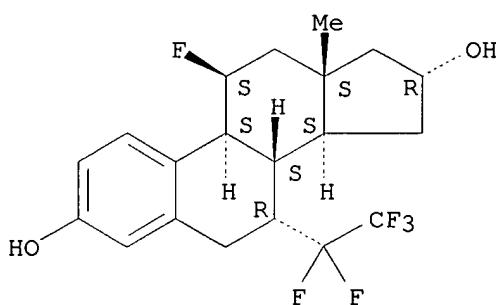
Absolute stereochemistry.



RN 287722-58-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(pentafluoroethyl)-,
(7. α .,11. β .,16. α .)- (9CI) (CA INDEX NAME)

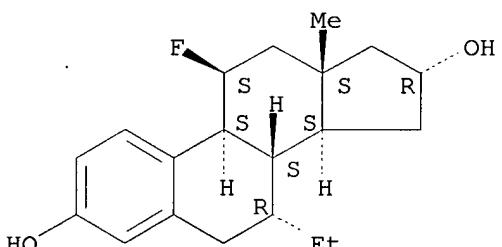
Absolute stereochemistry.



RN 287722-59-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7. α .,11. β .,16. α .)- (9CI) (CA INDEX NAME)

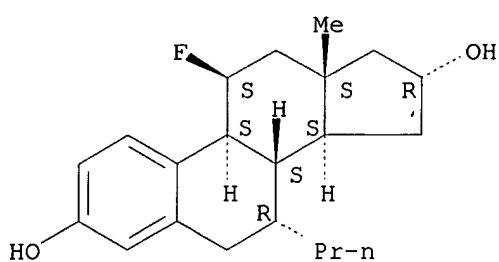
Absolute stereochemistry.



RN 287722-60-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7. α .,11. β .,16. α .)- (9CI) (CA INDEX NAME)

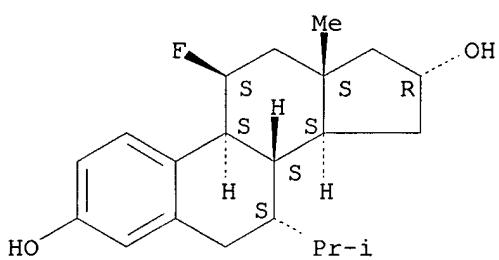
Absolute stereochemistry.



RN 287722-61-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

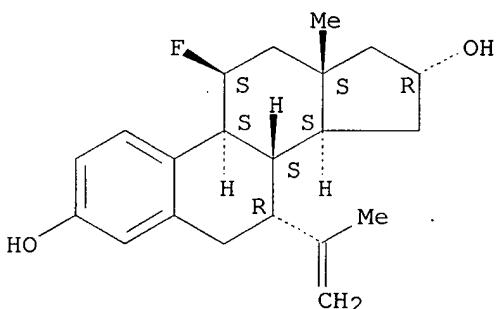
Absolute stereochemistry.



RN 287722-62-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

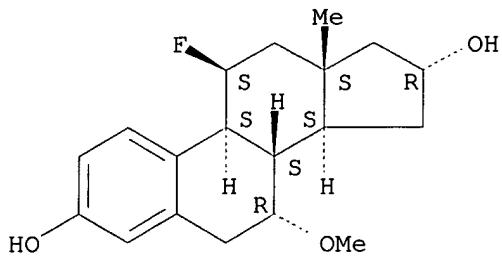
Absolute stereochemistry.



RN 287722-64-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

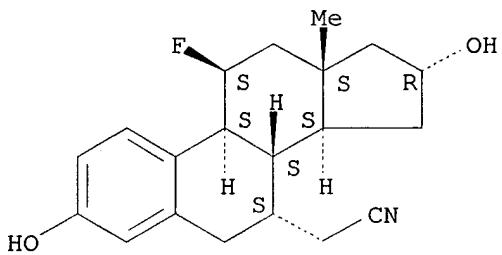
Absolute stereochemistry.



RN 287722-66-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7. α ,11. β ,16. α)-(9CI) (CA INDEX NAME)

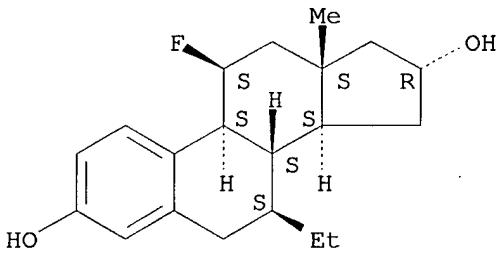
Absolute stereochemistry.



RN 287722-67-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-, (7. β ,11. β ,16. α)-(9CI) (CA INDEX NAME)

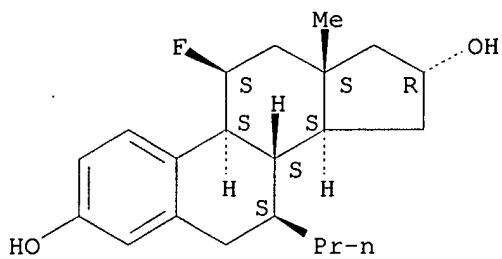
Absolute stereochemistry.



RN 287722-68-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-, (7. β ,11. β ,16. α)-(9CI) (CA INDEX NAME)

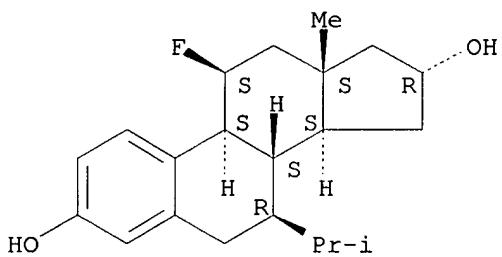
Absolute stereochemistry.



RN 287722-69-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.beta.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

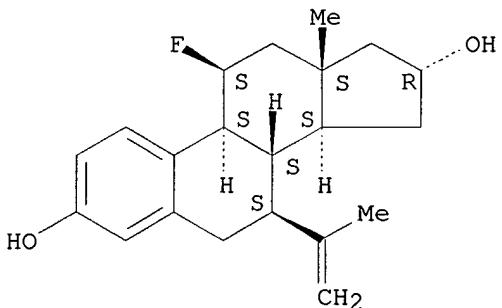
Absolute stereochemistry.



RN 287722-70-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.beta.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

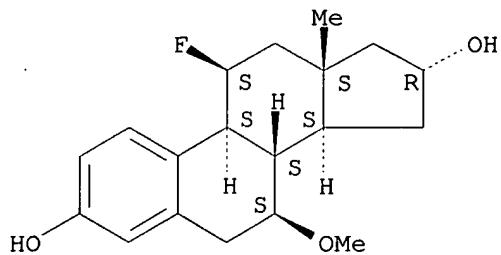
Absolute stereochemistry.



RN 287722-72-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.beta.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

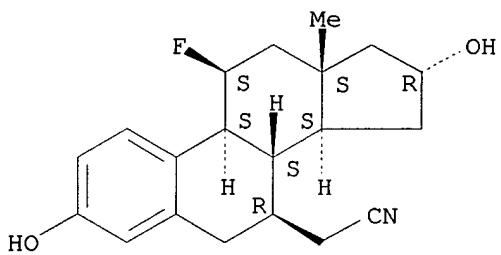
Absolute stereochemistry.



RN 287722-74-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7.β.,11.β.,16.α.)- (9CI) (CA INDEX NAME)

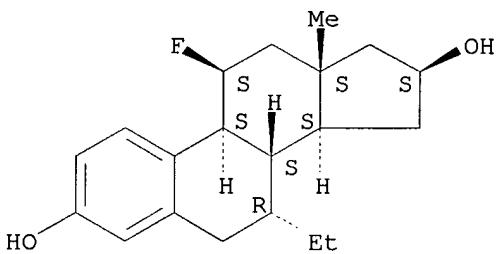
Absolute stereochemistry.



RN 287722-75-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7.α.,11.β.,16.β.)- (9CI) (CA INDEX NAME)

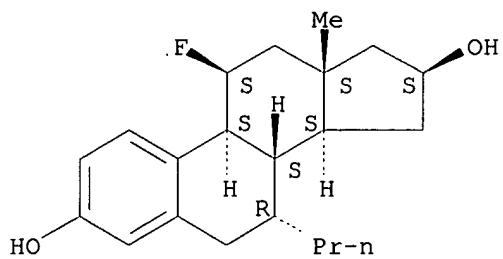
Absolute stereochemistry.



RN 287722-76-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7.α.,11.β.,16.β.)- (9CI) (CA INDEX NAME)

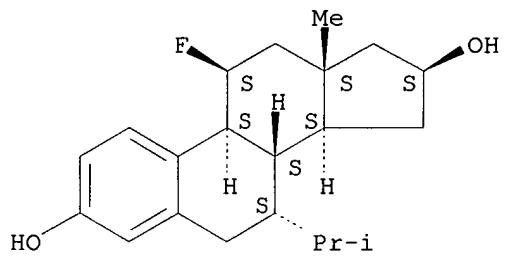
Absolute stereochemistry.



RN 287722-77-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-, (7. α .,11. β .,16. β .)- (9CI) (CA INDEX NAME)

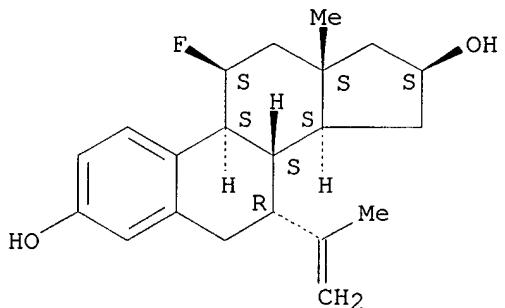
Absolute stereochemistry.



RN 287722-78-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-, (7. α .,11. β .,16. β .)- (9CI) (CA INDEX NAME)

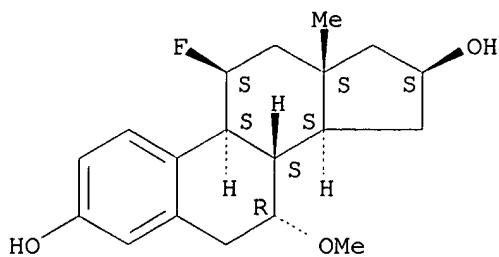
Absolute stereochemistry.



RN 287722-80-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-, (7. α .,11. β .,16. β .)- (9CI) (CA INDEX NAME)

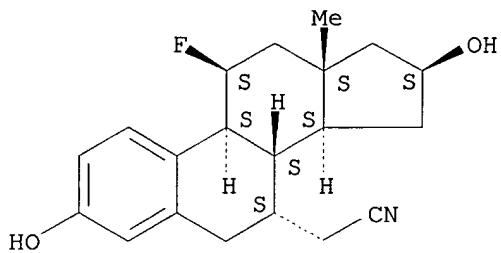
Absolute stereochemistry.



RN 287722-82-1 HCPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7. α ,11. β ,16. β)- (9CI) (CA INDEX NAME)

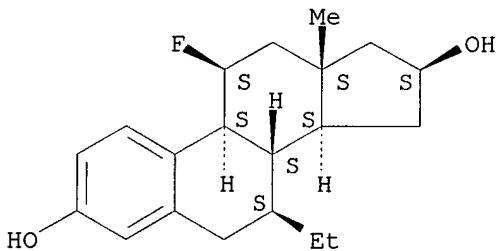
Absolute stereochemistry.



RN 287722-83-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-, (7. β ,11. β ,16. β)- (9CI) (CA INDEX NAME)

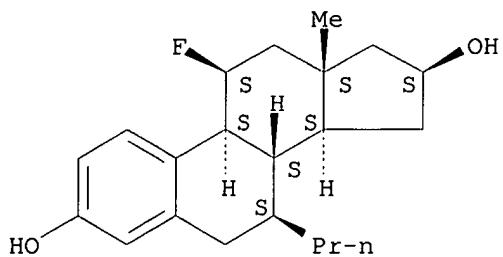
Absolute stereochemistry.



RN 287722-84-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-, (7. β ,11. β ,16. β)- (9CI) (CA INDEX NAME)

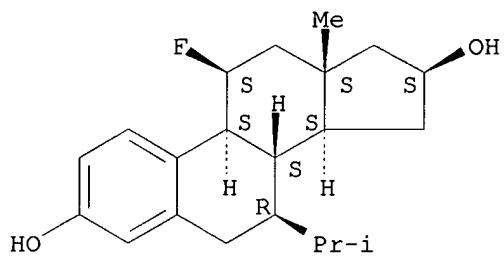
Absolute stereochemistry.



RN 287722-85-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.beta.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

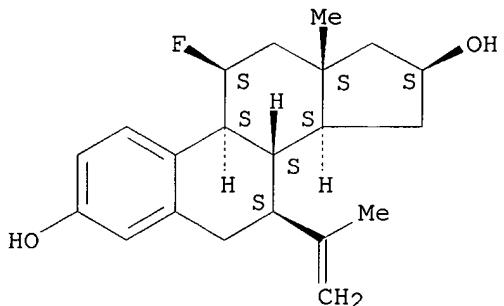
Absolute stereochemistry.



RN 287722-86-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.beta.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

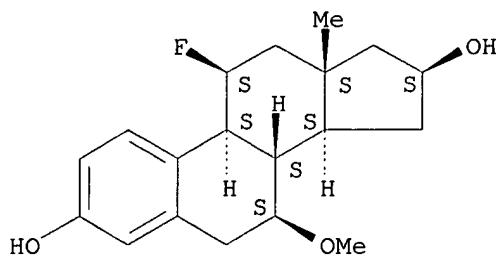
Absolute stereochemistry.



RN 287722-88-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.beta.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

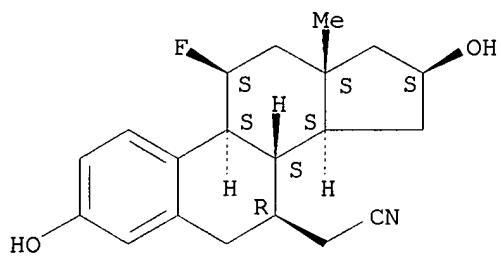
Absolute stereochemistry.



RN 287722-90-1 HCPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-, (7.β.,11.β.,16.β.)- (9CI) (CA INDEX NAME)

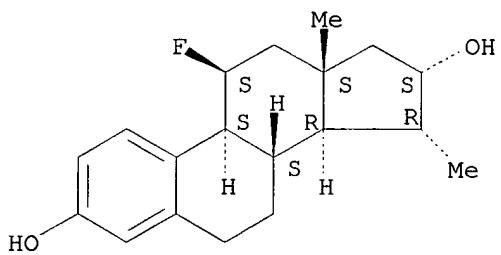
Absolute stereochemistry.



RN 287722-91-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-, (11.β.,15.α.,16.α.)- (9CI) (CA INDEX NAME)

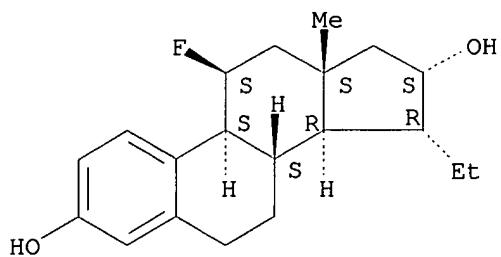
Absolute stereochemistry.



RN 287722-92-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-, (11.β.,15.α.,16.α.)- (9CI) (CA INDEX NAME)

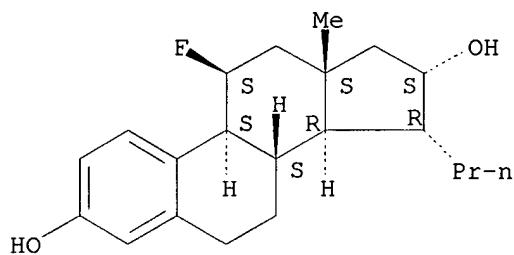
Absolute stereochemistry.



RN 287722-93-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11.β.,15.α.,16.α.)- (9CI) (CA INDEX NAME)

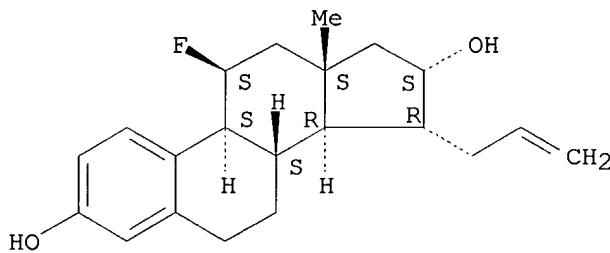
Absolute stereochemistry.



RN 287722-94-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.β.,15.α.,16.α.)- (9CI) (CA INDEX NAME)

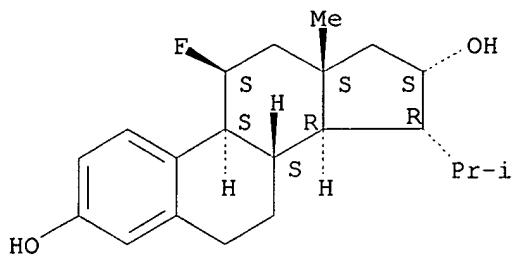
Absolute stereochemistry.



RN 287722-95-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.β.,15.α.,16.α.)- (9CI) (CA INDEX NAME)

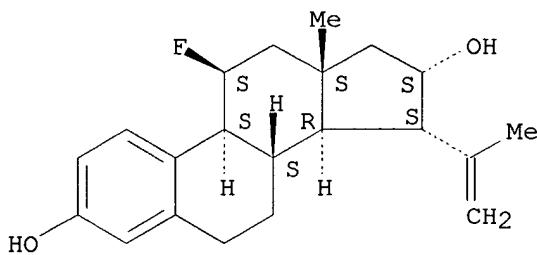
Absolute stereochemistry.



RN 287722-96-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11 beta.,15 alpha.,16 alpha.)- (9CI) (CA INDEX NAME)

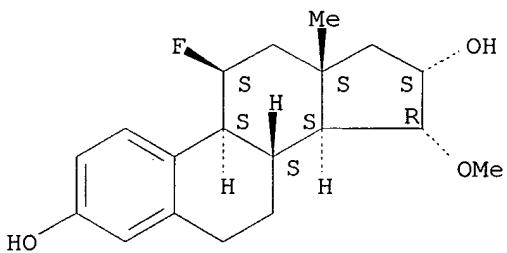
Absolute stereochemistry.



RN 287722-97-8 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11 beta.,15 alpha.,16 alpha.)- (9CI) (CA INDEX NAME)

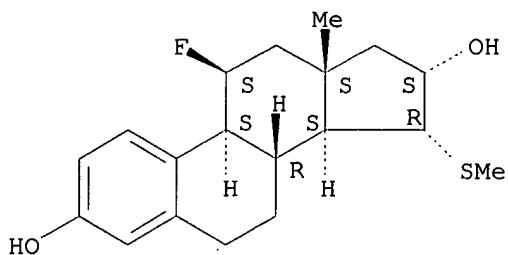
Absolute stereochemistry.



RN 287722-98-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11 beta.,15 alpha.,16 alpha.)- (9CI) (CA INDEX NAME)

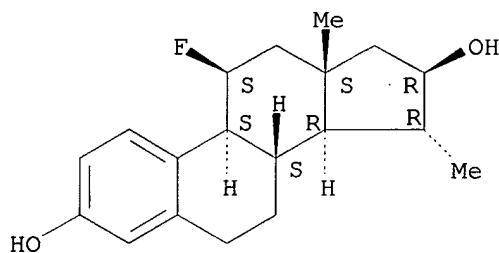
Absolute stereochemistry.



RN 287722-99-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-, (11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

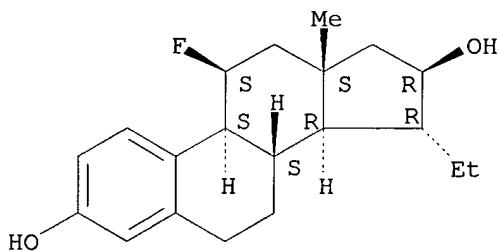
Absolute stereochemistry.



RN 287723-00-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-, (11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

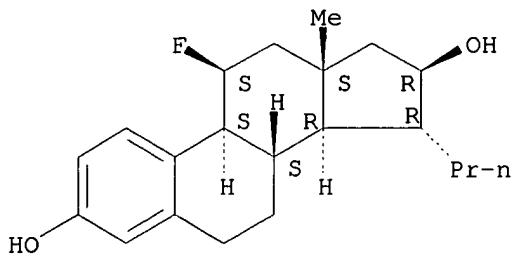
Absolute stereochemistry.



RN 287723-01-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-, (11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

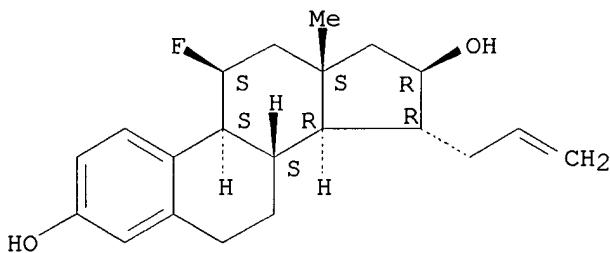
Absolute stereochemistry.



RN 287723-02-8 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

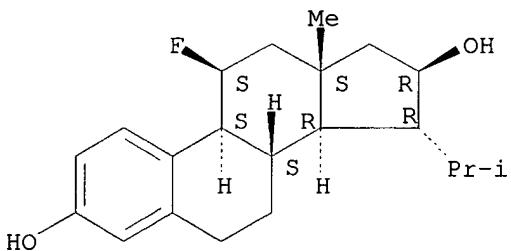
Absolute stereochemistry.



RN 287723-03-9 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

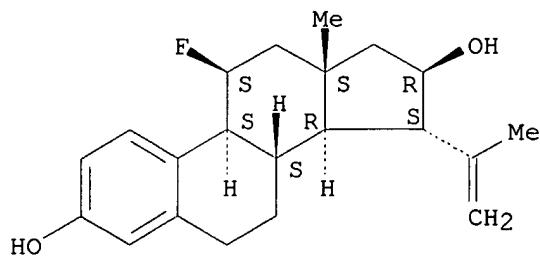
Absolute stereochemistry.



RN 287723-04-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

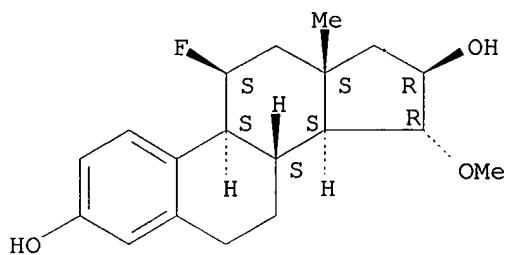
Absolute stereochemistry.



RN 287723-05-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
(11.β.,15.α.,16.β.)- (9CI) (CA INDEX NAME)

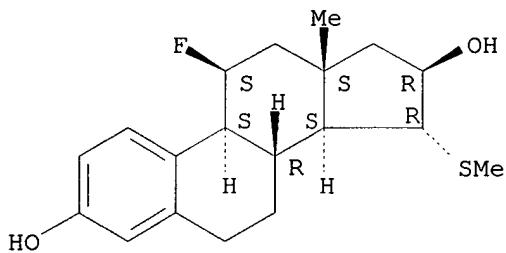
Absolute stereochemistry.



RN 287723-06-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
(11.β.,15.α.,16.β.)- (9CI) (CA INDEX NAME)

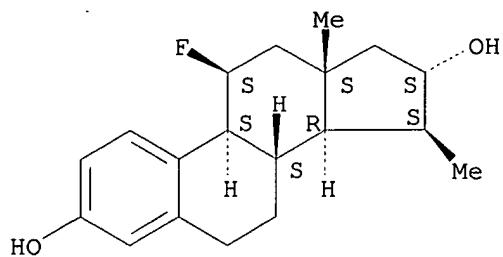
Absolute stereochemistry.



RN 287723-07-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
(11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

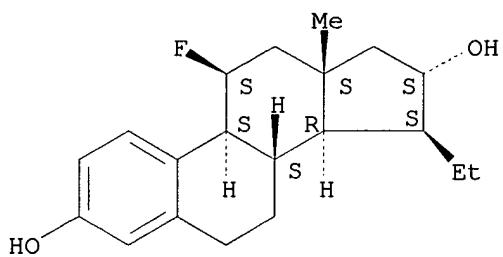
Absolute stereochemistry.



RN 287723-08-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
(11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

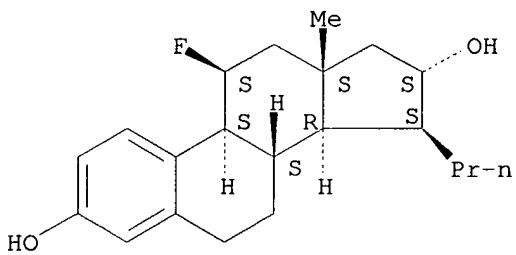
Absolute stereochemistry.



RN 287723-09-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

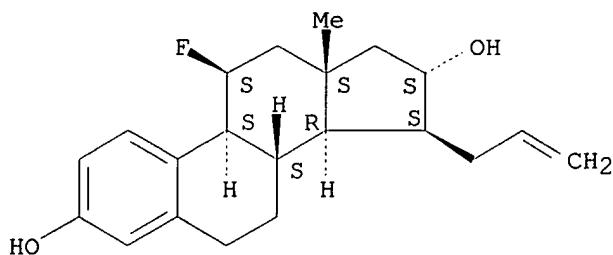
Absolute stereochemistry.



RN 287723-10-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

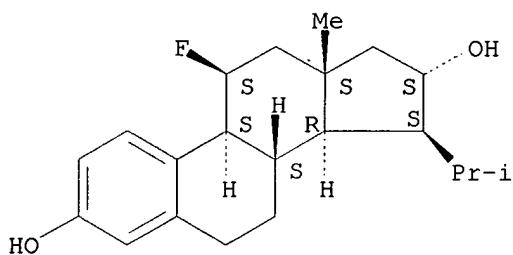
Absolute stereochemistry.



RN 287723-11-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-, (11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

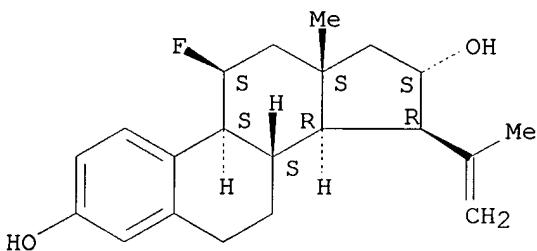
Absolute stereochemistry.



RN 287723-12-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

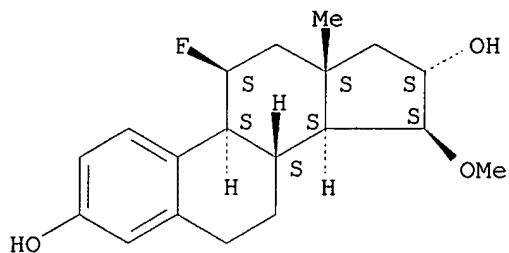
Absolute stereochemistry.



RN 287723-13-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-, (11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

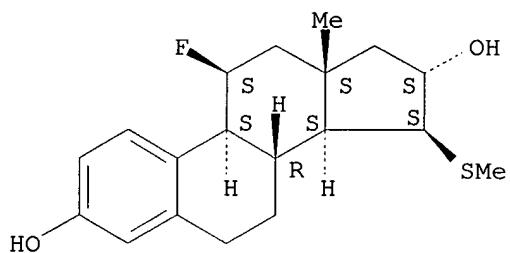
Absolute stereochemistry.



RN 287723-14-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
(11.betta.,15.betta.,16.alpha.)- (9CI) (CA INDEX NAME)

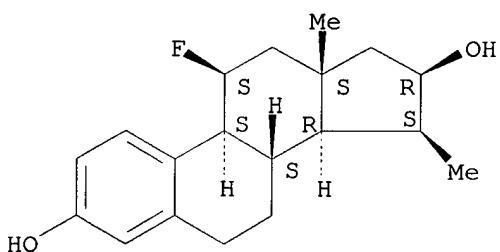
Absolute stereochemistry.



RN 287723-15-3 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
(11.betta.,15.betta.,16.betta.)- (9CI) (CA INDEX NAME)

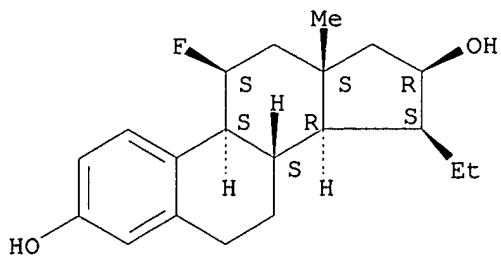
Absolute stereochemistry.



RN 287723-16-4 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
(11.betta.,15.betta.,16.betta.)- (9CI) (CA INDEX NAME)

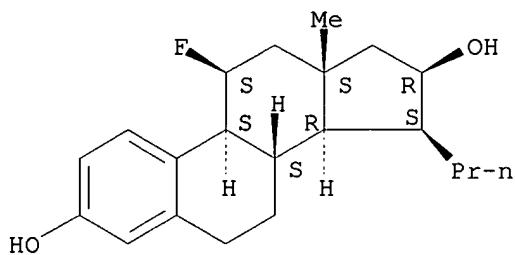
Absolute stereochemistry.



RN 287723-17-5 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

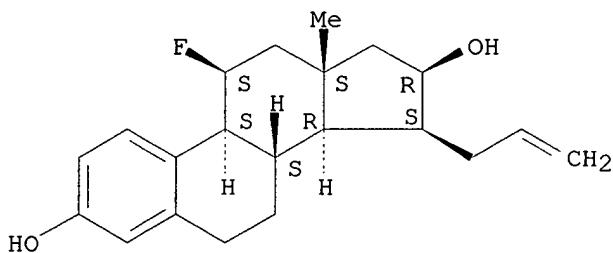
Absolute stereochemistry.



RN 287723-18-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

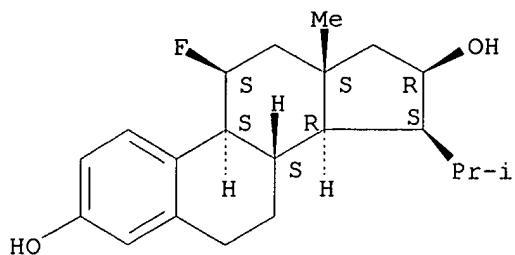
Absolute stereochemistry.



RN 287723-19-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

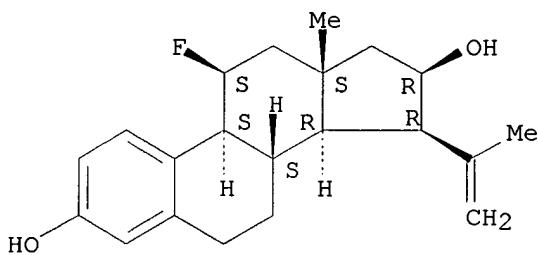
Absolute stereochemistry.



RN 287723-20-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-, (11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

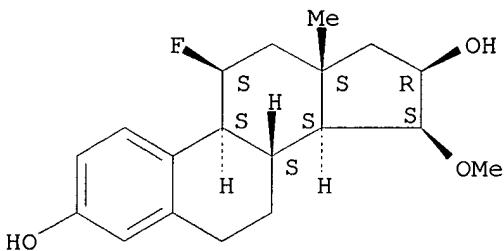
Absolute stereochemistry.



RN 287723-21-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-, (11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

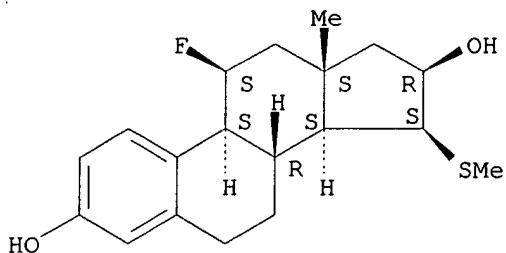
Absolute stereochemistry.



RN 287723-22-2 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-, (11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

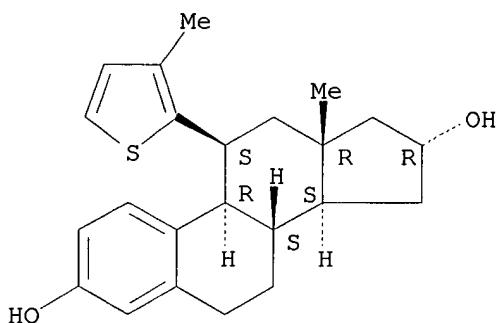
Absolute stereochemistry.



RN 287724-23-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-,
(11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

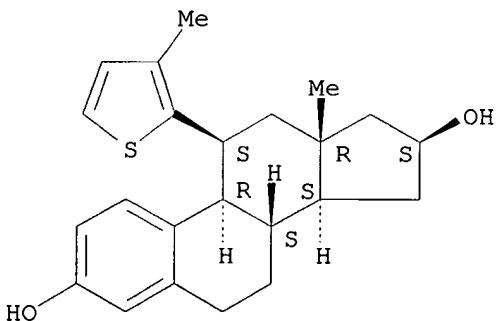
Absolute stereochemistry.



RN 287724-24-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-,
(11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



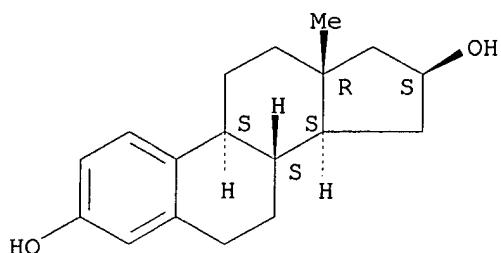
IT 1225-58-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 16-Hydroxyestratrienes as selectively effective
estrogens)

RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 7 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:648063 HCPLUS

DOCUMENT NUMBER: 131:332226

TITLE: Ligand structure influences autologous downregulation of estrogen receptor-alpha messenger RNA

AUTHOR(S): Davis, M. D.; VanderKuur, J. A.; Brooks, S. C.

CORPORATE SOURCE: Department of Biochemistry and Molecular Biology and the Barbara Ann Karmanos Cancer Institute, Wayne State University School of Medicine, Detroit, MI, 48201, USA

SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1999), 70(1-3), 27-37

CODEN: JSBBEZ; ISSN: 0960-0760

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of A- and D-ring substituted estrogen analogs have been examined for their effect on estrogen receptor-alpha (ER.alpha.) mRNA downregulation. Recently it has been proposed that ER.alpha. autologous downregulation occurs via transcriptional repression exerted by the binding of the ER.alpha.-ligand complex to the 5' region of the coding region of the ER.alpha. gene. Placement of the phenolic hydroxyl group on the various carbons of the arom. A-ring of estratrien-17.beta.-ol (carbons 1-3) produced ligands which diminished the steady state level of ER.alpha. mRNA in relation to their affinity for receptor. 4-Hydroxyestratrien-17.beta.ol, was inactive in the downregulation of ER.alpha. mRNA. Although this A-ring isomer brought about apparent processing of the nuclear receptor, the ER.alpha. reappeared in the cytosol within 24 h. Unlike the stimulation of genes regulated via estrogen response elements, max. autologous neg. regulation of the ER.alpha. gene required the presence of an hydroxyl group on carbon 17 of the D-ring. These results suggest that the conformational alterations elicited in the ER.alpha. mol. by various ligands create surfaces capable of interacting with other transcription factors in a manner which is different when the receptor functions via a response element mechanism relative to interactions during autologous neg. regulation of the ER.alpha. gene.

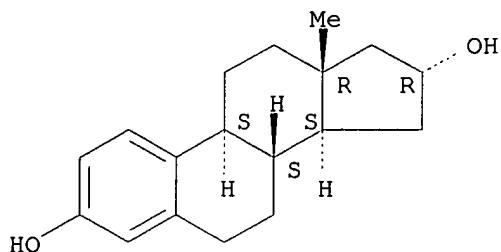
IT 1090-04-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(ligand structure influences autologous downregulation of estrogen receptor-.alpha. mRNA)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:424629 HCPLUS

DOCUMENT NUMBER: 131:223634

TITLE: The two phyto-estrogens genistein and quercetin exert different effects on estrogen receptor function

AUTHOR(S): Miodini, P.; Fioravanti, L.; Di Fronzo, G.; Cappelletti, V.

CORPORATE SOURCE: Istituto Nazionale per lo Studio e la Cura dei Tumori, Milan, Italy

SOURCE: British Journal of Cancer (1999), 80(8), 1150-1155
CODEN: BJCAAI; ISSN: 0007-0920

PUBLISHER: Churchill Livingstone

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors compared the estrogenic and anti-estrogenic properties of the two well-known phyto-estrogens, genistein and quercetin, on the estrogen-sensitive breast cancer cell line MCF-7. Genistein exerted a biphasic effect on growth of MCF-7 cells, stimulating at low and inhibiting at high concns., whereas quercetin was only growth inhibitory. At doses which did not inhibit cell growth, resp. 5 and 1 .mu.M, genistein and quercetin counteracted estrogen- and transforming growth factor-.alpha.-promoted cell growth stimulation. Furthermore, genistein promoted transcription of the estrogen-regulated genes pS2 and cathepsin-D, whereas quercetin interfered with the estrogen-induced expression of the proteins. In in vitro binding expts., genistein competed with estradiol for binding to the estrogen receptor (ER), but quercetin did not. Quercetin and genistein down-regulated cytoplasmic ER levels and promoted a tighter nuclear assocn. of the ER, but only genistein was able to up-regulate progesterone receptor protein levels. In gel mobility assays, ER preincubation with estradiol or with the two phyto-estrogens led to the appearance of the same retarded band, excluding differences between the various complexes in binding to the consensus sequence. The data allowed the authors to conclude that quercetin acts like a pure anti-estrogen, whereas genistein displays mixed agonist/antagonist properties, and to formulate a hypothesis on the possible mechanism of action of such phyto-estrogens.

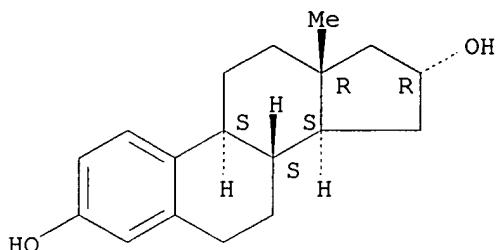
IT 1090-04-6, 16.alpha.-Estradiol

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(quercetin and genistein effect on growth of MCF-7 cell treated with estradiol and growth factors)

RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1999:407827 HCPLUS
 DOCUMENT NUMBER: 131:211611
 TITLE: Structure and toxicity of the cucurbitacins from Fevillea cordifolia
 AUTHOR(S): Echeverri, Fernando; Torres, Fernando; Lobo, Tatiana
 CORPORATE SOURCE: Department of Chemistry, Universidad de Antioquia, Medellin, Colombia
 SOURCE: Natural Product Analysis: Chromatography, Spectroscopy, Biological Testing, [Symposium], Wuerzburg, Germany, Sept. 1997 (1998), Meeting Date 1997, 385-386. Editor(s): Schreier, Peter. Vieweg: Wiesbaden, Germany.
 CODEN: 67USA7

DOCUMENT TYPE: Conference
 LANGUAGE: English

AB Several known fevicordins and two new cucurbitacins whose structures were assigned by 2D NMR were isolated from the seeds of Fevillea cordifolia. Although cucurbitacins are just recognized by their toxicity, the compds. isolated from F. cordifolia were i.p. inactive in mice at doses of 1.0 and 4.0 mg.

IT 151589-26-3 243139-36-8

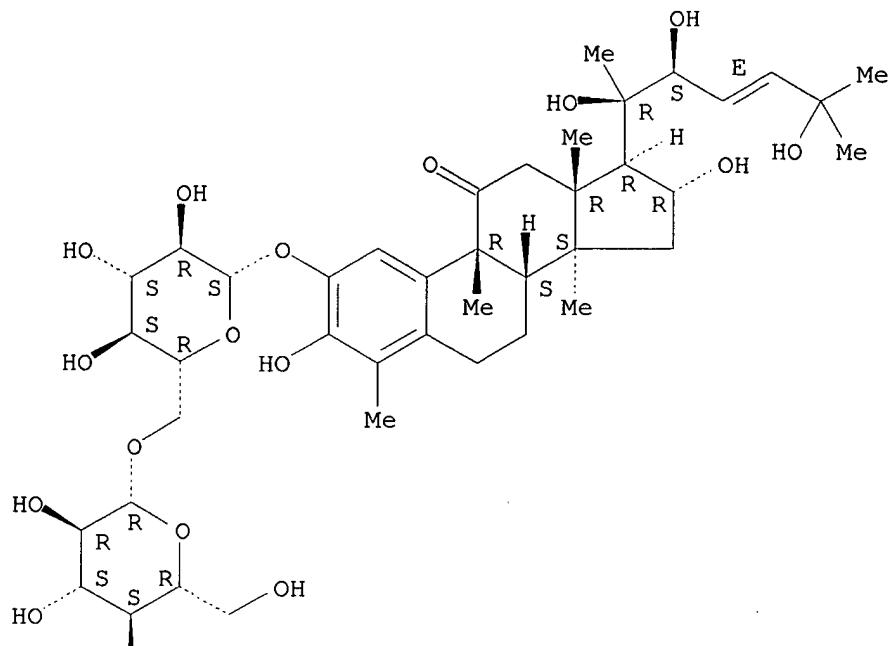
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
 (from Fevillea cordifolia)

RN 151589-26-3 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.

PAGE 1-A



PAGE 2-A

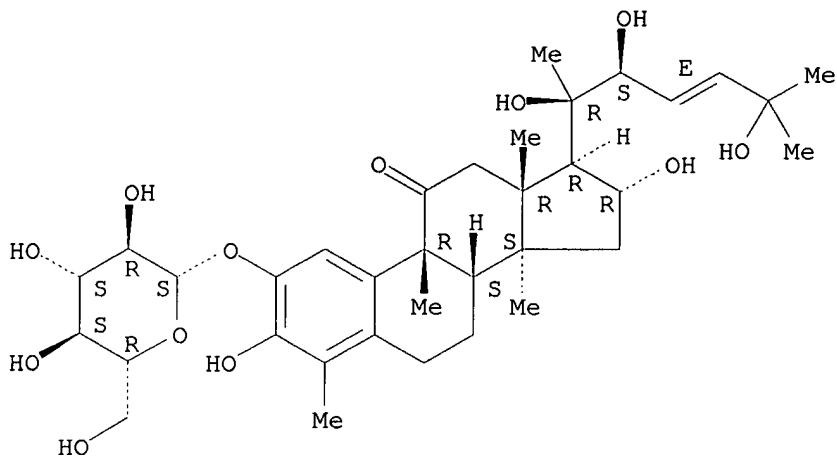


RN 243139-36-8 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



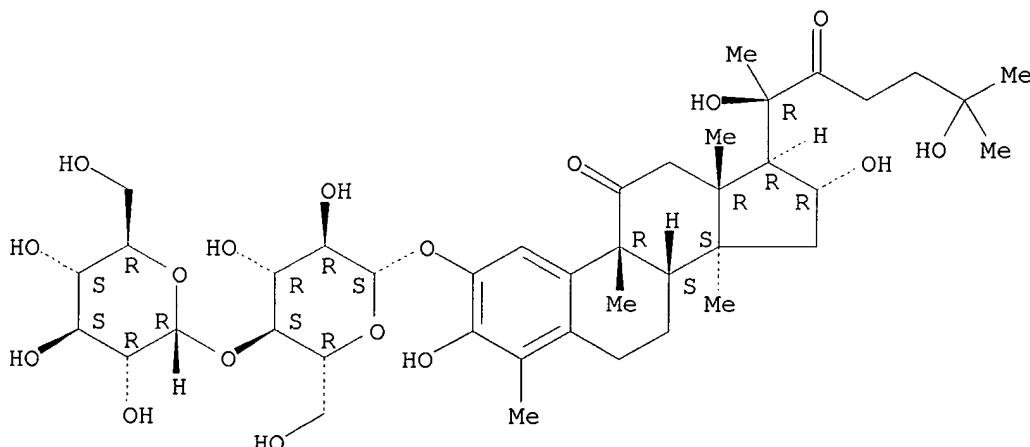
IT 243116-46-3P 243116-47-4P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(from Fevillea cordifolia)

RN 243116-46-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-[(4-O-.alpha.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,25-tetrahydroxy-4,9,14-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

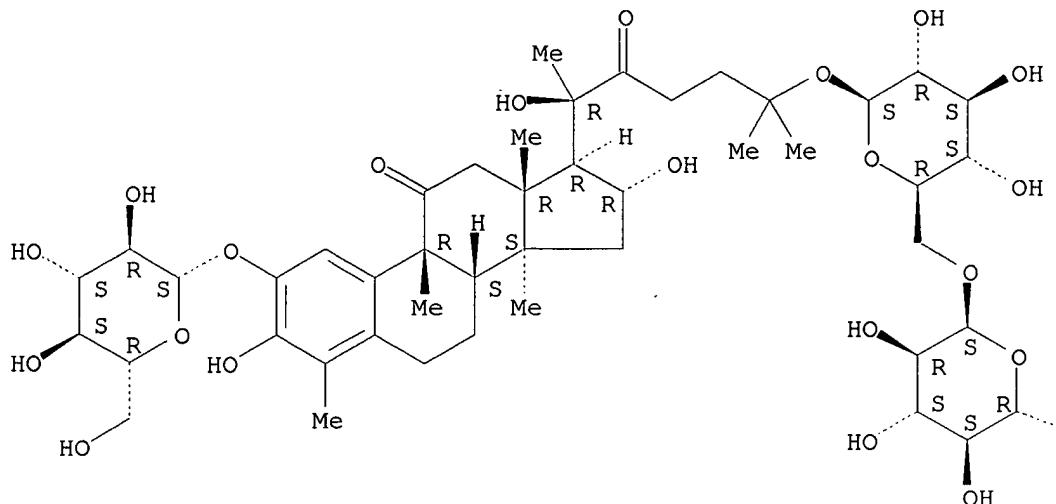


RN 243116-47-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-[(6-O-.alpha.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L5 ANSWER 10 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:559789 HCAPLUS

DOCUMENT NUMBER: 129:306174

TITLE: Analysis of potential endocrine disrupting chemicals
in sewage effluents using continuous liquid-liquid
extraction with derivatization and gas
chromatography/mass spectrometry analysisAUTHOR(S): Barber, Larry B.; Brown, Greg K.; Writer, Jeffery H.;
Zaugg, S. A.

CORPORATE SOURCE: U. S. Geological Survey, Boulder, CO, 80303, USA

SOURCE: Preprints of Extended Abstracts presented at the ACS
National Meeting, American Chemical Society, Division
of Environmental Chemistry (1998), 38(2), 273-275

CODEN: PEACF2

PUBLISHER: American Chemical Society, Division of Environmental Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Anal. of potential endocrine disrupting chems. in wastewater effluent using continuous liq.-liq. extn. with derivatization and gas chromatog./mass spectrometry anal. is described.

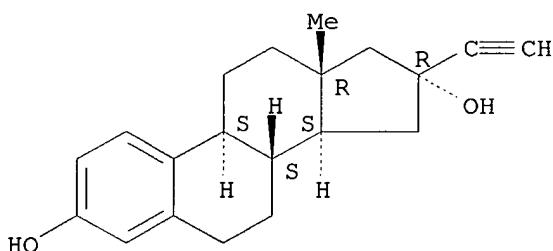
IT 24989-47-7

RL: ANT (Analyte); ANST (Analytical study)
(endocrine disrupting chems. detn. in wastewater by continuous liq.-liq. extn. with derivatization and gas chromatog./mass spectrometry anal. under base, neutral, and acid conditions)

RN 24989-47-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 16-ethynyl-, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:638466 HCPLUS

DOCUMENT NUMBER: 127:288310

TITLE: Induction of the Estrogen Specific Mitogenic Response of MCF-7 Cells by Selected Analogs of Estradiol-17.beta.: A 3D QSAR Study

AUTHOR(S): Wiese, Thomas E.; Polin, Lisa A.; Palomino, Eduardo; Brooks, S. C.

CORPORATE SOURCE: Department of Biochemistry, Wayne State University School of Medicine, Detroit, MI, 48201, USA

SOURCE: Journal of Medicinal Chemistry (1997), 40(22), 3659-3669

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Analogs of estradiol-17.beta. (E2) have been evaluated for estrogen receptor (ER) binding affinity and mitogenic potential in the human breast cancer cell line MCF-7. These 42 compds. represent subtle modifications of the natural estrogen structure through the placement of hydroxyl, amino, nitro, or iodo groups around the ring system in addn. to, or as replacement of, the 3- and 17.beta.-hydroxyls of E2. The mitogenic activity of the analogs was found to be related to ER binding only to a limited extent. To elucidate structural features that are uniquely responsible for receptor binding affinity or mitogen potential of estrogens, the three-dimensional quant. structure-activity (QSAR) method

Comparative Mol. Field Anal. (CoMFA) was employed. Sep. CoMFA models for receptor binding and cell growth stimulation were optimized through the use of various alignment rules and region step size. Whereas the CoMFA contour plots did outline the shared structural requirements for the two measured biol. properties, specific topol. features in this set of estrogens were delineated that distinguish mitogenic potential from ER binding ability. In particular, steric interference zones which affected growth extend in a band from above the A-ring to position 4 and below, whereas the ER binding steric interference zones are limited to isolated polyhedra in the 1,2 and 4 positions and the .alpha. face of the B-ring. In addn., electroneg. features located around the A-, B-, or C-rings contribute to receptor affinity. However, growth is dependent only on electroneg. and electropos. properties near the 3-position. In a final QSAR model for the mitogenic response, the value of ER binding was included along with structural features as a descriptor in CoMFA. The resulting 3D-QSAR has the most predictive potential of the models in this study and can be considered a prototype model for the general evaluation of a steroidal estrogen's growth stimulating ability in MCF-7 cells. For example, the location of D-ring contours illustrate the model's preference for 17.beta.-hydroxy steroids over the less mitogenic 17.alpha.- and 16.alpha.-hydroxy compds. In addn., the enhanced mitogenic effect of steric bulk in the 11.alpha.-position is also evident. The QSAR studies in this report illustrate the fact that while ER binding may be a required factor of the estrogen dependent growth response in MCF-7 cells, particular structural characteristics, in addn. to those responsible for tight receptor binding, must be present to induce an optimal mitogenic response. Therefore, this report demonstrates that the CoMFA QSAR method can be utilized to characterize structural features of test compds. that account for different types of estrogenic responses.

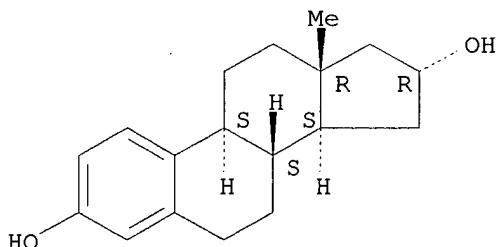
IT 1090-04-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (3D QSAR study of induction of estrogen specific mitogenic response of MCF-7 cells by selected analogs of estradiol)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 12 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:244398 HCPLUS

DOCUMENT NUMBER: 126:225448

TITLE: Novel estrogens for treating autoimmune diseases

INVENTOR(S): Brattsand, Ralph; Holmdahl, Rikard; Jansson, Liselotte; Loncar, Marjana; Pettersson, Lars

PATENT ASSIGNEE(S): Astra Aktiebolag, Swed.; Brattsand, Ralph; Holmdahl, Rikard; Jansson, Liselotte; Loncar, Marjana; Pettersson, Lars
 SOURCE: PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9708188	A1	19970306	WO 1996-SE1028	19960820
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
CA 2228803	AA	19970306	CA 1996-2228803	19960820
AU 9668405	A1	19970319	AU 1996-68405	19960820
EP 847399	A1	19980617	EP 1996-928771	19960820
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
JP 11511457	T2	19991005	JP 1997-510174	19960820
US 6043236	A	20000328	US 1997-817683	19970423
PRIORITY APPLN. INFO.:			SE 1995-2921	A 19950823
			WO 1996-SE1028	W 19960820

OTHER SOURCE(S): MARPAT 126:225448

AB Estratrienes I [R = H, alkyl, cycloalkyl, acyl, alkoxy carbonyl, aralkoxy carbonyl, protective group; R1, R2 = H, Me, Et, halogen; R3 = H, acyl, alkoxy carbonyl, aralkoxy carbonyl; R4 = H, Me, Et; Y = CH₂, bond] were prepd. Thus, estrone was converted to its 3-dimethylhexyl ether which was treated with Et₃PPh₃⁺ Br⁻, followed by SeO₂-Me₃COOH oxidn. and desilylation to give (17E)-3,16.alpha.-dihydroxy-19-norpregna-1,3,5(10),17(20)-tetraene. It shows very low sex hormone side effects while retaining their antiinflammatory and immunosuppressant activity.

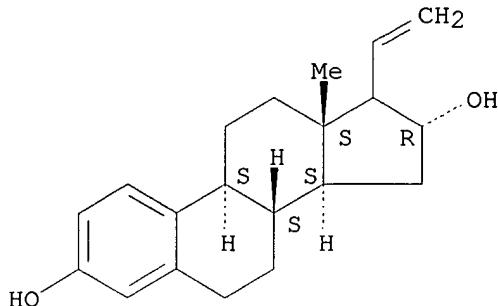
IT 188291-28-3P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of estratriene derivs. as inflammation inhibitors and immunosuppressants)

RN 188291-28-3 HCPLUS

CN 19-Norpregna-1,3,5(10),20-tetraene-3,16-diol, (16.alpha.,17.xi.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 13 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:683463 HCAPLUS

DOCUMENT NUMBER: 126:57556

TITLE: Geodisterol, a novel polyoxygenated sterol with an aromatic A ring from the tropical marine sponge *Geodia* sp.

AUTHOR(S): Wang, Gui-Yang-Sheng; Crews, Phil

CORPORATE SOURCE: Dep. Chem. and Biochem., Univ. of California, Santa Cruz, CA, 95064, USA

SOURCE: Tetrahedron Letters (1996), 37(45), 8145-8146
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Geodisterol (I), the first marine polyoxygenated sterol with an arom. A ring, was isolated from the Indo-Pacific sponge *Geodia* sp. The structural and stereochem. features of I were based on the extensive anal. of 1D and 2D of it and MPA esters.

IT 185146-75-2P

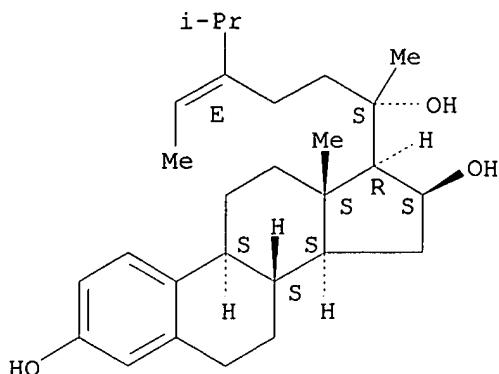
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(geodisterol isolation and structural characterization from tropical marine sponge)

RN 185146-75-2 HCAPLUS

CN 19-Norstigmasta-1,3,5(10),24(28)-tetraene-3,16,20-triol, (16.beta.,24E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



L5 ANSWER 14 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:449391 HCAPLUS

DOCUMENT NUMBER: 125:81803

TITLE: Studies on the Constituents of Cyclanthera pedata
(Caigua) Seeds: Isolation and Characterization of Six
New Cucurbitacin Glycosides

AUTHOR(S): De Tommasi, Nunziatina; De Simone, Francesco; Pizza,
Cosimo

CORPORATE SOURCE: Facolta di Farmacia, Universita di Salerno, Penta di
Fisciano, 84084, Italy

SOURCE: Journal of Agricultural and Food Chemistry (1996),
44(8), 2020-2025

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Six new cucurbitacin glycosides were isolated from the seeds of Cyclanthera pedata Schrab (Cucurbitaceae). Their structures were elucidated on the basis of spectral and chem. data to be 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16.alpha.,20,22,25-pentahydroxy-29-norcucurbita-1,3,5(10)-trien-11-one, 25-acetoxy-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16.alpha.,20,22-tetrahydroxy-29-norcucurbita-1,3,5(10)-trien-11-one, 25-acetoxy-2-(.beta.-D-glucopyranosyloxy)-3,16.alpha.,20,22-tetrahydroxy-29-norcucurbita-1,3,5(10)-trien-11-one, 25-acetoxy-2-[(4-O-.alpha.-L-rhamnopyranosyl-6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16.alpha.,20-trihydroxy-29-norcucurbita-1,3,5(10)-triene-11,22-dione, 3.beta.-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-16.alpha.,20,22,25-tetrahydroxycucurbit-5-en-11-one, and 3-.beta.-(.beta.-D-glucopyranosyloxy)-25-acetoxy-16.alpha.,20,22,-trihydroxycucurbit-5-en-11-one.

IT 178062-90-3P 178062-91-4P 178062-92-5P

178062-93-6P

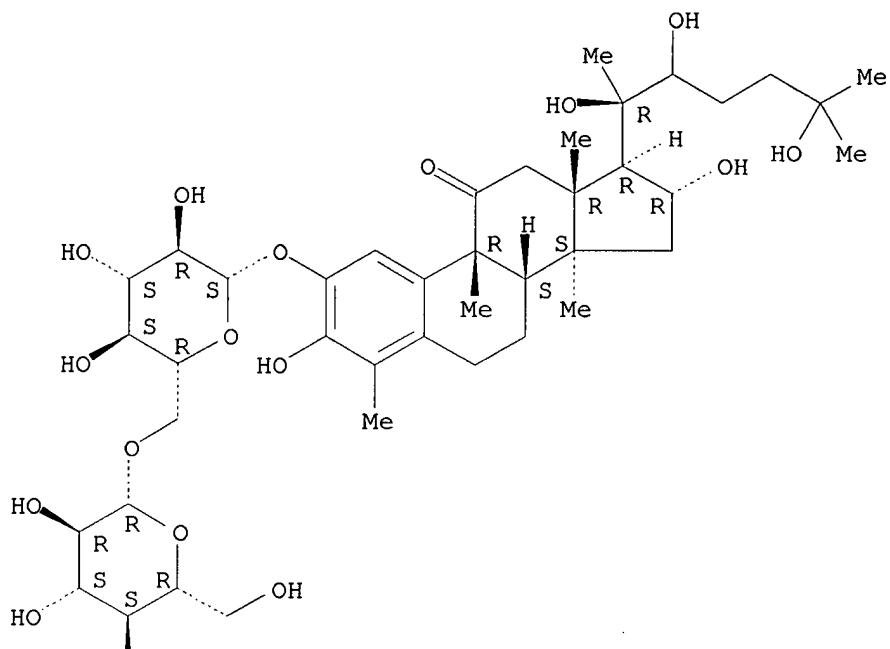
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation from Cyclanthera pedata seeds and structure of)

RN 178062-90-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22-tetrahydroxy-25-hydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A

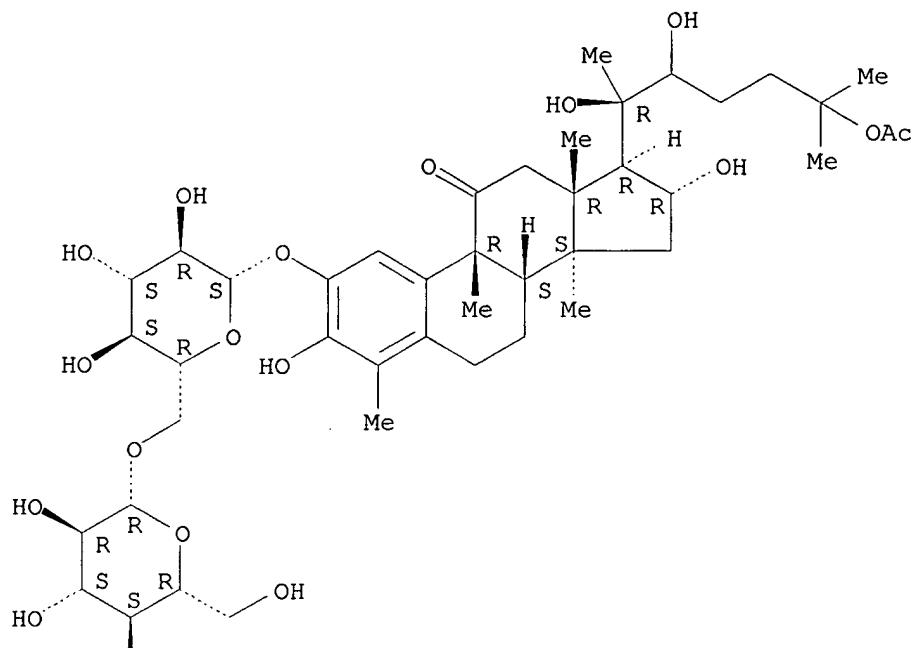


RN 178062-91-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 25-(acetyloxy)-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



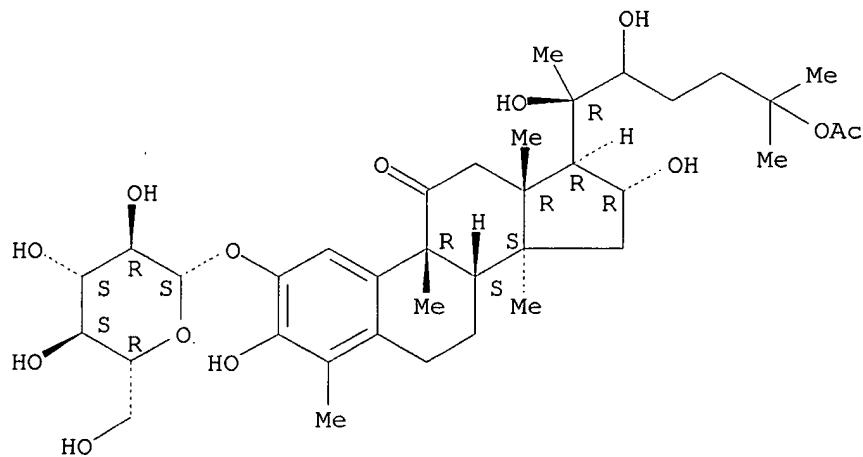
PAGE 2-A

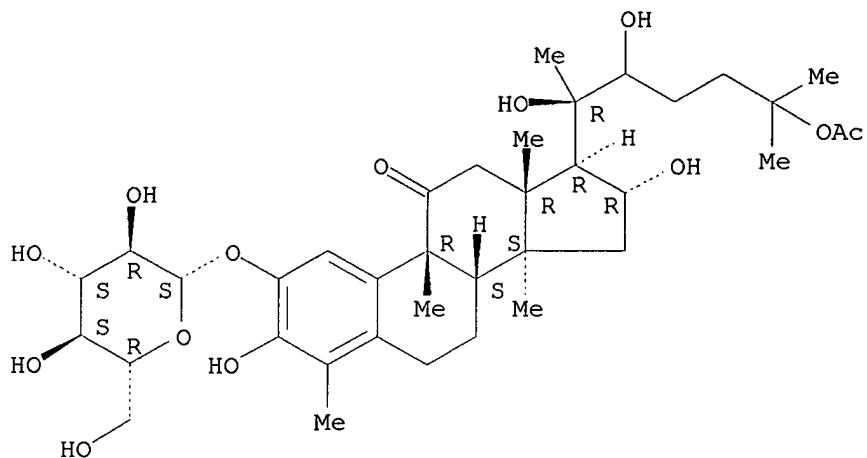


RN 178062-92-5 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



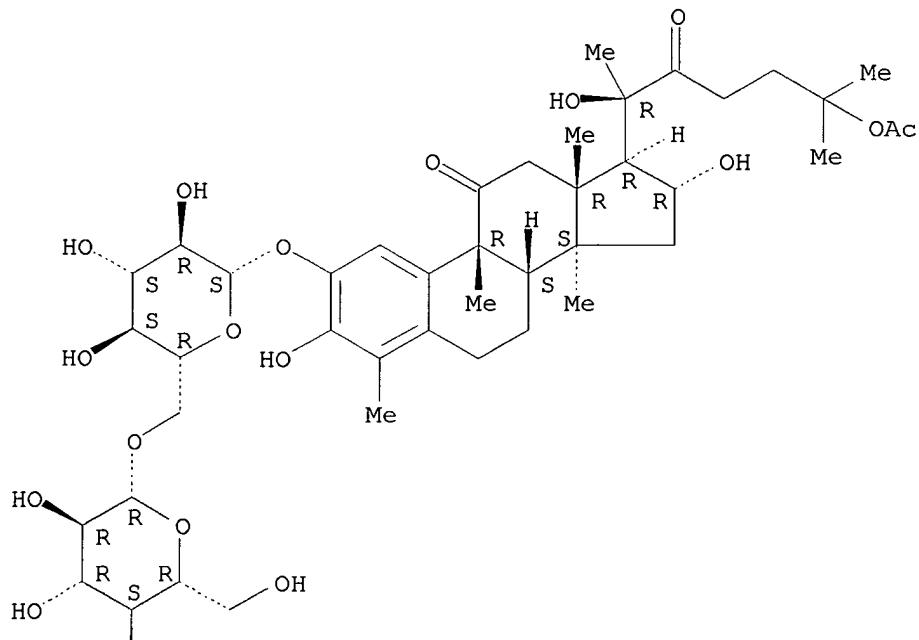


RN 178062-93-6 HCPLUS

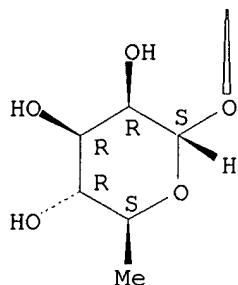
CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-[(O-6-deoxy-alpha.-L-mannopyranosyl-(1.fwdarw.4))-O-.beta.-D-glucopyranosyl-(1.fwdarw.6)-.beta.-D-glucopyranosyl]oxy]-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A



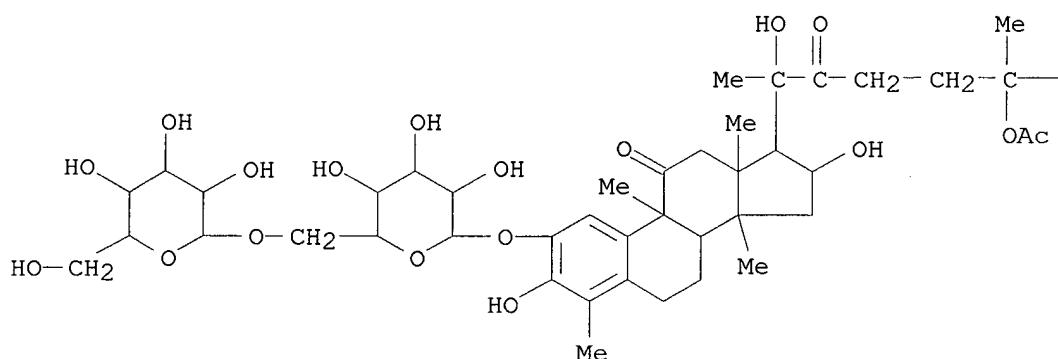
IT 151589-22-9

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 BIOL (Biological study); OCCU (Occurrence)
 (of Cyclanthera pedata seeds)

RN 151589-22-9 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— Me

L5 ANSWER 15 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:901632 HCAPLUS

DOCUMENT NUMBER: 123:306774

TITLE: Relationship between estrogen structure and conformational changes in estrogen receptor/DNA complexes

AUTHOR(S): Christman, J. K.; Nehls, S.; Polin, L.; Brooks, S. C.

CORPORATE SOURCE: Molecular Biology Program, Michigan Cancer Foundation, Detroit, MI, 48201, USA

SOURCE: Journal of Steroid Biochemistry and Molecular Biology

(1995), 54(5/6), 201-10
 CODEN: JSBBEZ; ISSN: 0960-0760

PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The effect of estrogen structure on the conformation of the complex formed with estrogen receptor (ER) and the consensus estrogen response element (EREc) has been examd. with gel mobility shift assay. Proteins in MCF-7 cell exts. formed three distinct complexes with ERE. Only the slowest moving complex contained ER as indicated by binding with anti-ER antibodies H222 and D547. This ER-ERE complex displayed increased electrophoretic mobility when formed in the presence of estradiol (E2) and bound radiolabeled 16.alpha.-iodoestradiol. The antiestrogen ICI 164384 decreased the mobility of the ER-ERE complex and blocked the effect of E2. The results reported here indicate that the position and location of hydroxyl groups on the estratriene nucleus is an important factor in detg. the mobility of ER-EREc (or a variant ERE) in gel shift assays. The ability of E2 analogs to cause conformational changes detectable as altered mobility was not directly related either to their binding affinity for ER or to their ability to activate E2 responsive genes. Although several dihydroxy estrogens (estradiol-16.alpha., 1- and 2-hydroxyestratrien-17.beta.-ol) caused an increased in the mobility of the ER-EREc, other ligands (estradiol-17.alpha., 4-hydroxyestratrien-17.beta.-ol, 3-hydroxyestratriene, estratrien-17.beta.-ol and 5-androstene-3.beta.,17.beta.-diol) with a capacity for activating at least some E2 responsive genes in MCF-7 cells had little or no effect. On the basis of these and previously published results, it can be concluded that specific structures of estrogens are responsible for conformational changes of ER-ERE complexes detectable in gel-shift assays. Furthermore, the identified structural characteristics of the ligand which are required for gel-shift are not the same as those previously reported to be essential for stimulation of transcriptional activity of ER.

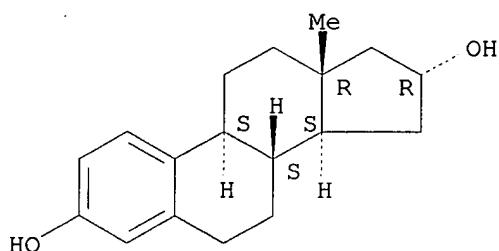
IT 1090-04-6, 16.alpha.-Estradiol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (estrogen structure in relation to conformational changes in estrogen receptor-estrogen-responsive element complexes)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 16 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1995:766521 HCPLUS
 DOCUMENT NUMBER: 123:222777

TITLE: Constituents of tropical medicinal plants. LXVII:
24-Acetylaminofevicordin D glucoside, an artificial
constituent of Fevillea cordifolia? On the reactivity
of fevicordins

AUTHOR(S): Achenbach, Hans; Horn, Konrad; Waibel, Reiner

CORPORATE SOURCE: Institut Pharmazie lebensmittelchemie, Universitaet
Erlangen, Erlangen, 91052, Germany

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1995),
328(6), 481-5

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: German

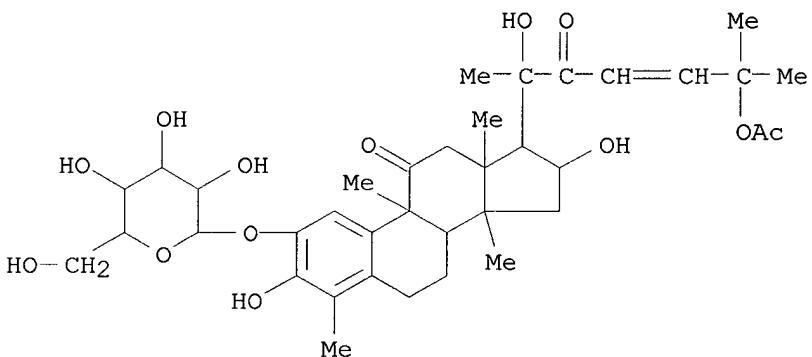
AB 24-Acetylaminofevicordin D glucoside (I) was isolated as a minor component from the seeds of Fevillea cordifolia (Cucurbitaceae) and its structure was detd. by spectroscopic methods. Expts. showed that the enone-system in the side chain of fevicordin A glucoside, which represents the main constituent of the seeds, undergoes a Michael addn. with nucleophiles, and ammonia reacts very easily under simultaneous migration of the acetyl group from C-25 to the nitrogen. Therefore, I probably has to be regarded as an artifact.

IT 111250-01-2, Fevicordin A glucoside

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(Michael addn. and NMR data and reactivity of)

RN 111250-01-2 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-,
(9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)



IT 168287-72-7P 168287-76-1P

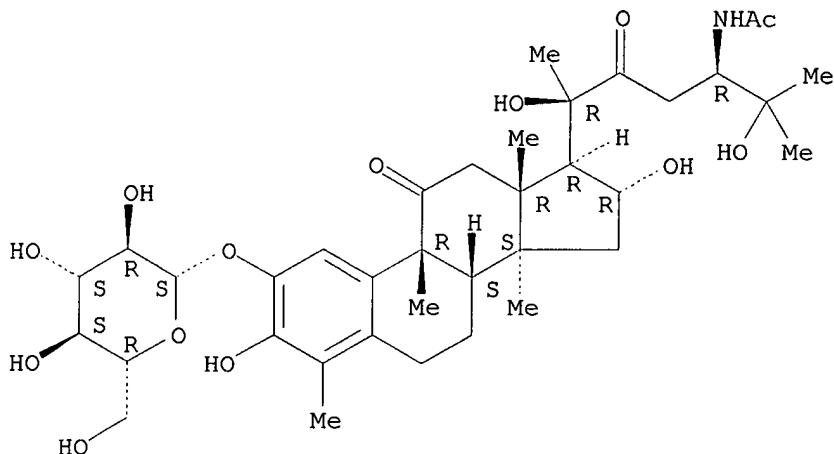
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); FMU
(Formation, unclassified); PRP (Properties); RCT (Reactant); SPN
(Synthetic preparation); BIOL (Biological study); FORM (Formation,
nonpreparative); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or
reagent)

(isolation as artifact from Fevillea and NMR data and prepn. and
acetylation of)

RN 168287-72-7 HCPLUS

CN Acetamide, N-[(9.beta.,16.alpha.,24R)-2-(.beta.-D-glucopyranosyloxy)-
3,16,20,25-tetrahydroxy-4,9,14-trimethyl-11,22-dioxo-19-norcholesta-
1,3,5(10)-trien-24-yl]- (9CI) (CA INDEX NAME)

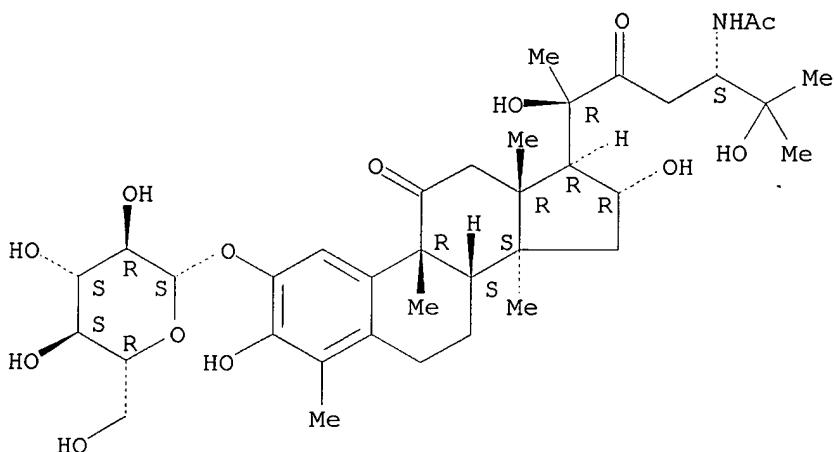
Absolute stereochemistry. Rotation (-).



RN 168287-76-1 HCAPLUS

CN Acetamide, N-[(9.beta.,16.alpha.,24S)-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-11,22-dioxo-19-norcholest-1,3,5(10)-trien-24-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



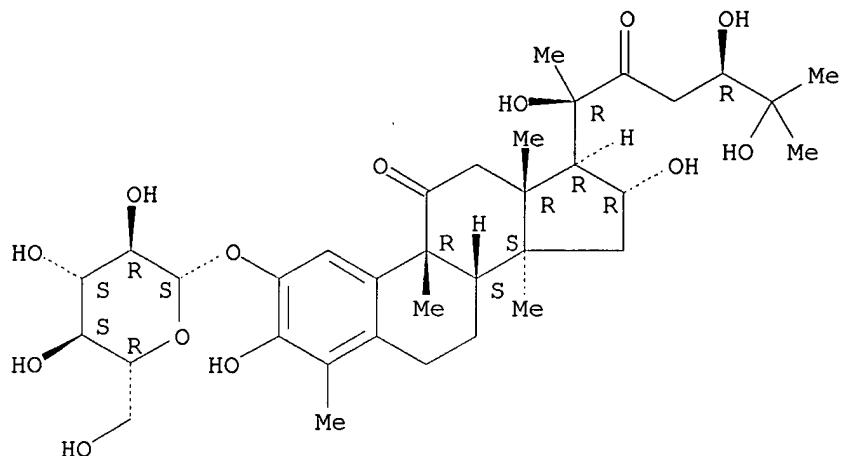
IT 168287-73-8P 168287-77-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prep. and NMR data of)

RN 168287-73-8 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,24,25-pentahydroxy-4,9,14-trimethyl-,
(9.beta.,16.alpha.,24R)- (9CI) (CA INDEX NAME)

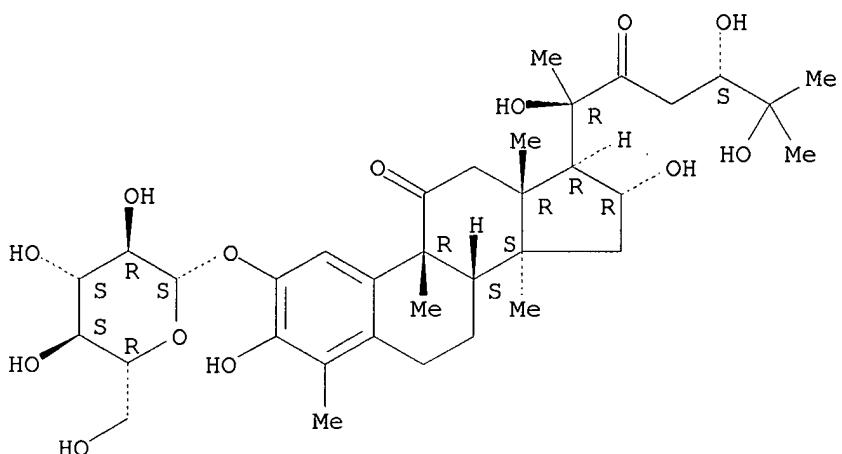
Absolute stereochemistry.



RN 168287-77-2 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,24,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



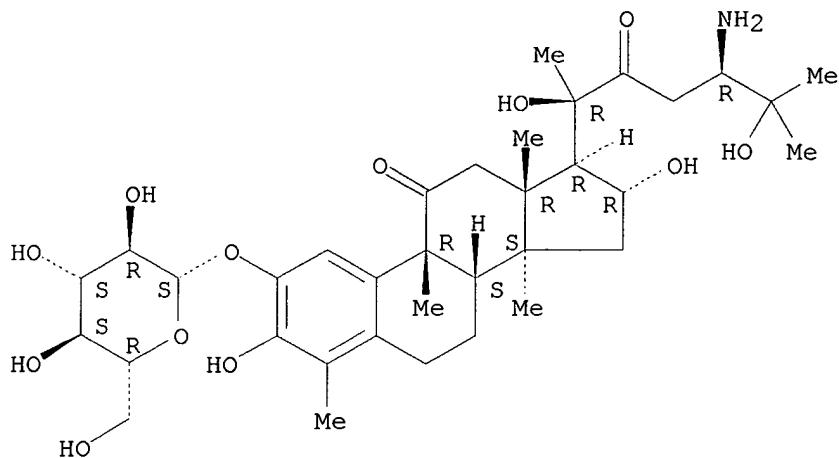
IT 168287-74-9P 168287-78-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prep. and acetylation and NMR data of)

RN 168287-74-9 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 24-amino-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24R)- (9CI) (CA INDEX NAME)

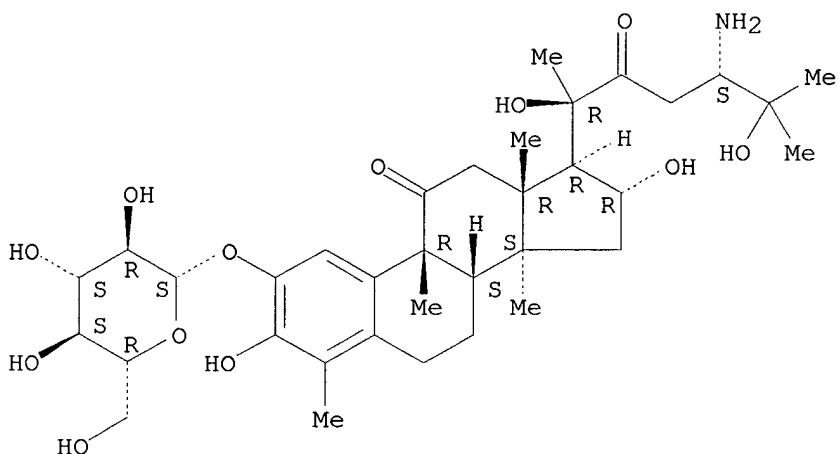
Absolute stereochemistry.



RN 168287-78-3 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 24-amino-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 151589-19-4P

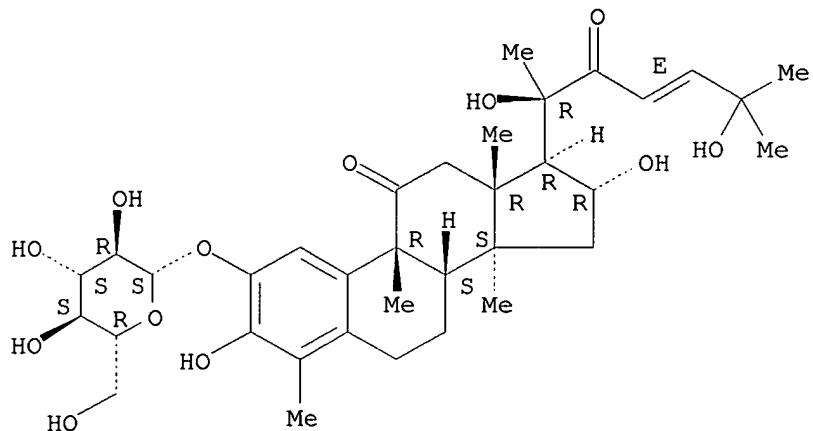
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prep. and reactions with ammonia and KOH)

RN 151589-19-4 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L5 ANSWER 17 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:651424 HCAPLUS

DOCUMENT NUMBER: 123:48115

TITLE: Cellular localization of estradiol-induced c-fos messenger ribonucleic acid in the rat uterus: c-fos expression and uterine cell proliferation do not correlate strictly

AUTHOR(S): Nephew, Kenneth P.; Peters, Gregory A.; Khan, Sohaib A.

CORPORATE SOURCE: Coll. Med., Univ. Cincinnati, Cincinnati, OH, 45267-0521, USA

SOURCE: Endocrinology (1995), 136(7), 3007-15
CODEN: ENDOAO; ISSN: 0013-7227

PUBLISHER: Endocrine Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Estrogens stimulate DNA synthesis and cell proliferation in the uterus. All major uterine cell types (luminal and glandular epithelium, stroma, and myometrium) respond to 17. β -estradiol in the immature animal, whereas primarily epithelia cells of the uterine endometrium respond in the mature animal. Rapid activation of the c-fos protooncogene by estrogen precedes the uterine growth, suggesting that c-fos plays a role in amplifying the hormonal signal. The specific uterine cell types in which estrogen induces c-fos mRNA expression, however, have not been identified in either mature or immature animals. In this study, *in situ* hybridization was used to det. the cell type-specific location of mRNA encoding c-fos in the uterus. In both immature and mature castrated rats at 3 h after 17. β -estradiol administration, c-fos expression was detected primarily in uterine luminal and glandular epithelia. Expression of c-fos returned to baseline levels by 24 h post 17. β -estradiol treatment. There was no apparent difference in the uterine cell type-specific pattern of c-fos expression stimulated by estradiol in mature vs. immature animals. Nuclear run-on transcription assay is isolated luminal epithelial cell nuclei showed that c-fos gene transcription increased rapidly in the uterus after estradiol stimulation. Treatment of adult rats with a single injection of 16. α -estradiol, a short-acting, nonmitogenic estrogen, induced c-fos primarily in the uterine glandular epithelia. Progesterone is known to modify the action of estrogen on the uterus by redirecting the proliferative response from

epithelia to stroma. To det. if progesterone modulation of estrogen action involves shifting of c-fos expression to stromal cells, rats were treated with progesterone for 48 h and then killed 0, 3, 6, or 12 h after an estradiol injection. In situ hybridization anal. revealed that c-fos mRNA remained localized in the uterine luminal and a glandular epithelia, and expression was not shifted to the stroma. Although these results support the idea that c-fos plays a role in proliferation of uterine epithelial cells, they also invite reassessment of the role played by c-fos in both epithelial and nonepithelial uterine cell types.

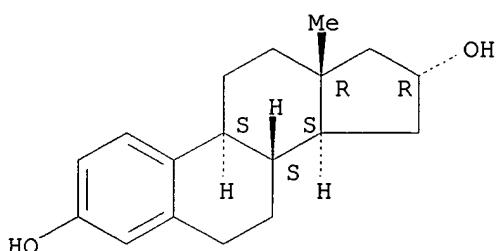
IT 1090-04-6, 16.alpha.-Estradiol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(cellular localization of estradiol-induced c-fos mRNA in uterus in relation to cell proliferation)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 18 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:585753 HCPLUS

DOCUMENT NUMBER: 122:306705

TITLE: Induction of tissue plasminogen activator mRNA and activity by structurally altered estrogens

AUTHOR(S): Davis, M. D.; Butler, W. B.; Brooks, S. C.

CORPORATE SOURCE: Dep. Biochemistry, Wayne State Univ. School Medicine, USA

SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1995), 52(5), 421-30

CODEN: JSBBEZ; ISSN: 0960-0760

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of structure of the estrogen ligand on the accumulation of tPA mRNA and the activity of extracellular fibrinolytic enzyme has been examd. in cultures of MCF-7 cells. Estradiol (E2)-stimulated fibrinolytic activity was preceded by an increase in actinomycin D sensitive tPA mRNA synthesis which peaked at 18 h. Ten A- and D-ring structural analogs of E2 affected tPA mRNA accumulation and extracellular fibrinolytic activity. Only in the case of two A-ring isomers (2- and 4-hydroxyestratrien-17.beta.-ol) was the decreased effect of the ligand's structural change on tPA mRNA accumulation and fibrinolysis not explained by a comparable decline in affinity of the ligand for estrogen receptor. Both of these analogs functioned as antiestrogens. The stimulatory capacity of

androstanediols on the tPA gene required that the 3-hydroxyl group be positioned in the .beta.-configuration. Absence of the 17.beta.-hydroxy group was beneficial to the max. accumulation of tPA mRNA. As has been reported for other estrogen responsive genes (progesterone receptor, cathepsin D and pS2), regulation by estrogens is not related directly to the affinity of the ligand for ER, but this activity may be detd. by the location of the electroneg. isopotential above the A-ring of estrogenic ligands.

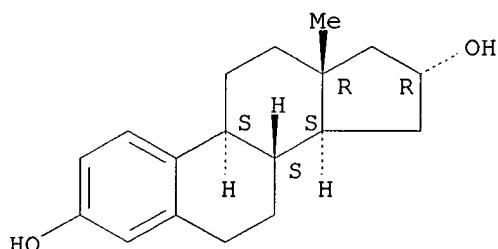
IT 1090-04-6, 16.alpha.-Estradiol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(tissue plasminogen activator induction by structurally altered estrogens)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 19 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:441845 HCPLUS

DOCUMENT NUMBER: 122:281523

TITLE: Inhibitory effects of cucurbitane triterpenoids on Epstein-Barr virus activation and two-stage carcinogenesis of skin tumor. II

AUTHOR(S): Konoshima, Takao; Takasaki, Midori; Kozuka, Mutsuo; Nagao, Tsuneatsu; Okabe, Hikaru; Irino, Nobuto; Nakasumi, Tetsuo; Tokuda, Harukuni; Nishino, Hoyoku

CORPORATE SOURCE: Kyoto Pharm. Univ., Kyoto, 607, Japan

SOURCE: Biological & Pharmaceutical Bulletin (1995), 18(2), 284-7

CODEN: BPBLEO; ISSN: 0918-6158

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To search for possible anti-tumor-promoters, we carried out a primary screening of twenty-four 29-nor-cucurbitacin glucosides isolated from the roots of Cayaponia tayuya (Cucurbitaceae) using an in vitro synergistic assay system. Of these glucosides, cayaponosides B (5), B3 (7), D (8), D3b (22) and C2 (23) exhibited significant inhibitory effects on Epstein-Barr virus (EBV) activation induced by the tumor promoter, 12-O-tetradecanoylphorbol-13-acetate (TPA). Furthermore, 5 and 23 exhibited remarkable anti-tumor-promoting effects on mouse skin tumor promotion in an in vivo two-stage carcinogenesis test.

IT 147742-04-9, Cayaponoside A 147742-05-0, Cayaponoside B

147742-06-1, Cayaponoside C 147764-94-1, Cayaponoside D

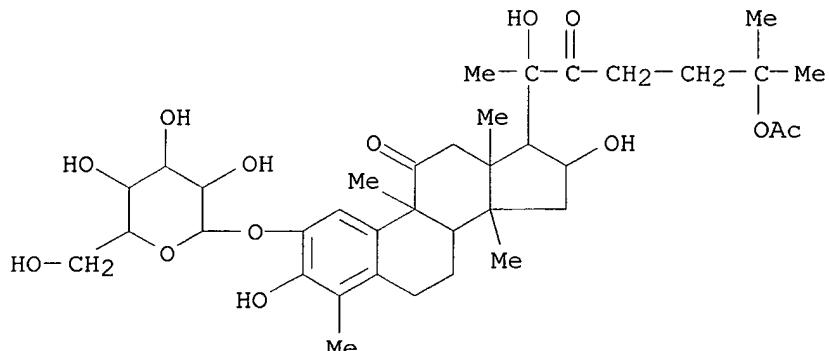
151589-19-4, Cayaponoside C5a **151703-09-2**, Cayaponoside B4 **151703-10-5**, Cayaponoside C2 **162857-56-9**, Cayaponoside A3 **162857-57-0**, Cayaponoside A4 **162857-58-1**, Cayaponoside A6 **162857-59-2**, Cayaponoside B2 **162857-60-5**, Cayaponoside B3 **162857-61-6**, Cayaponoside D1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(cucurbitane triterpenoids inhibition of Epstein-Barr virus and two-stage carcinogenesis of skin tumor)

RN 147742-04-9 HCPLUS

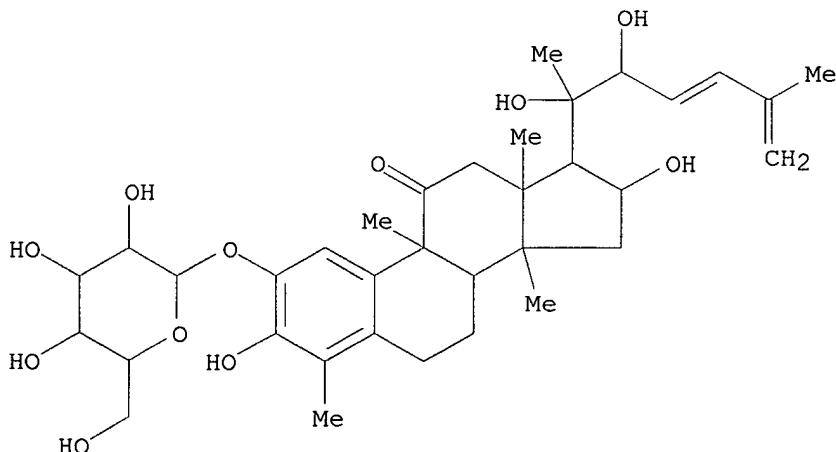
CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 147742-05-0 HCPLUS

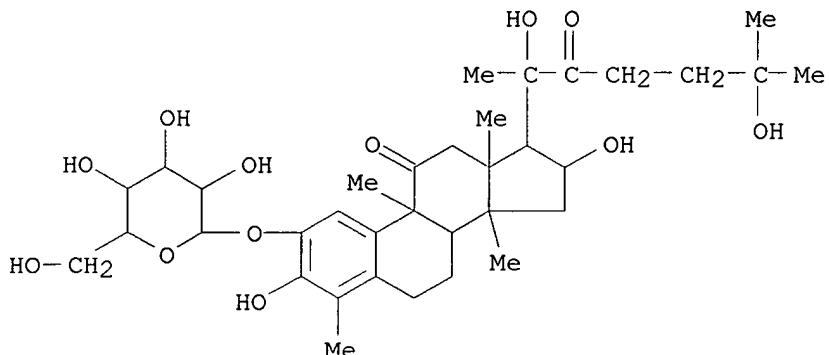
CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 147742-06-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



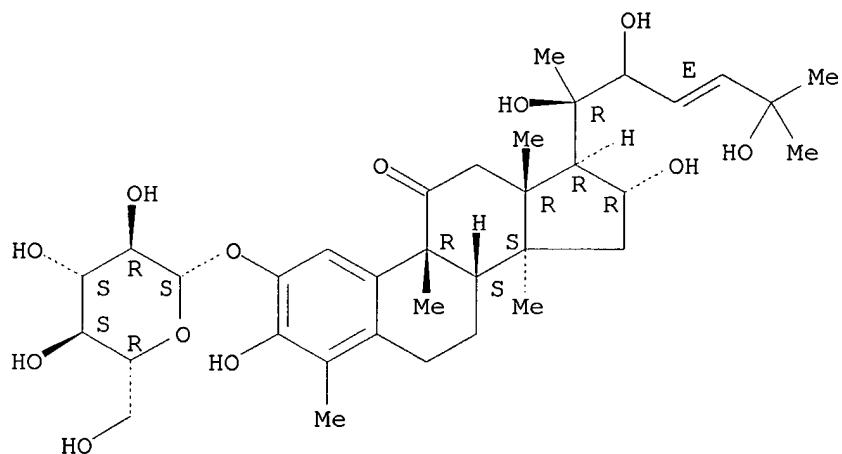
RN 147764-94-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Currently available stereo shown.

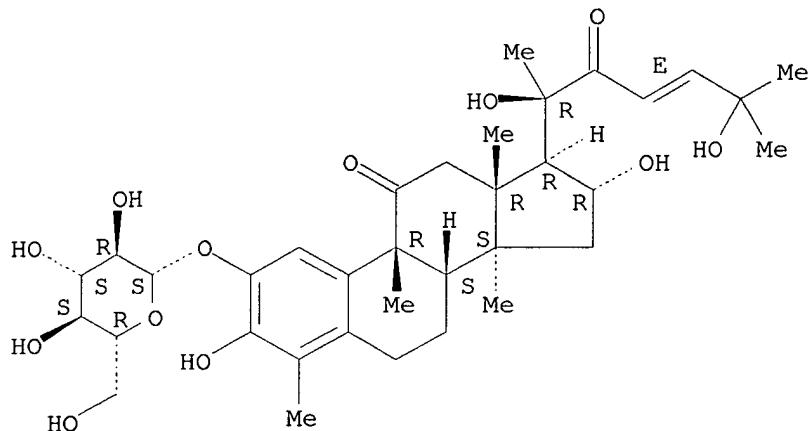


RN 151589-19-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

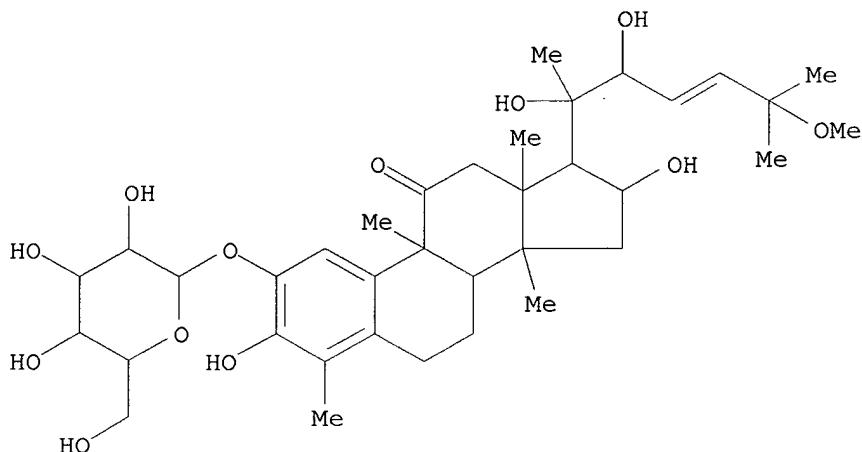
Double bond geometry as shown.



RN 151703-09-2 HCAPLUS

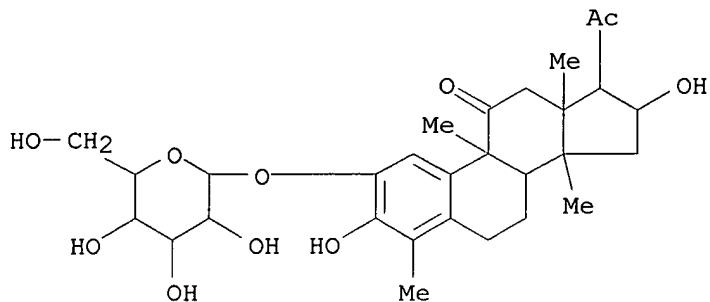
CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 151703-10-5 HCAPLUS

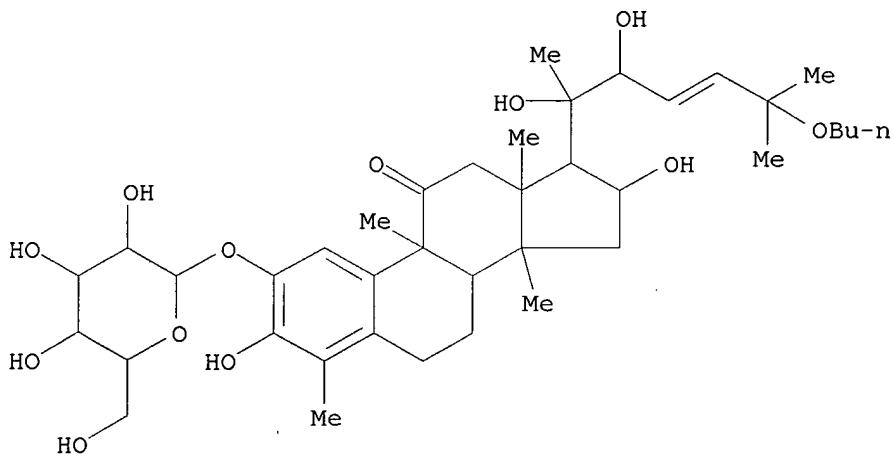
CN 19-Norpregna-1,3,5(10)-triene-11,20-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16-dihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 162857-56-9 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 25-butoxy-2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

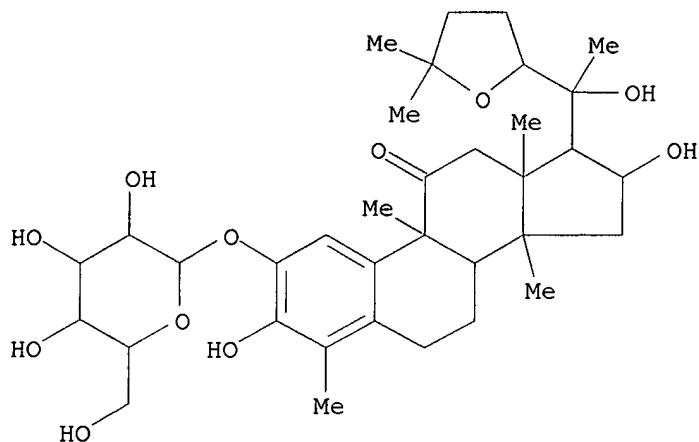
Currently available stereo shown.



RN 162857-57-0 HCPLUS

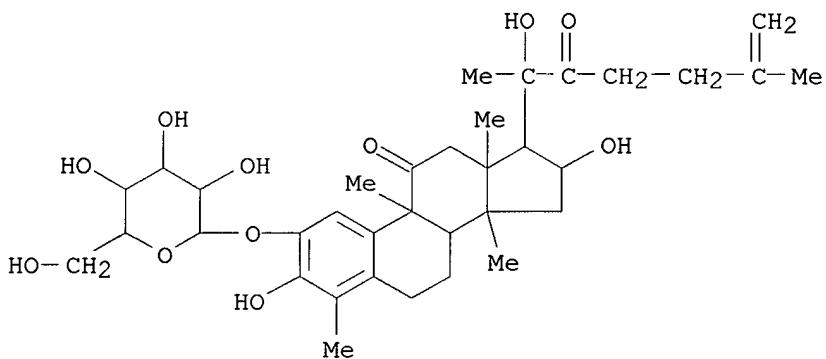
CN 19-Norcholesta-1,3,5(10)-trien-11-one, 22,25-epoxy-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 162857-58-1 HCAPLUS

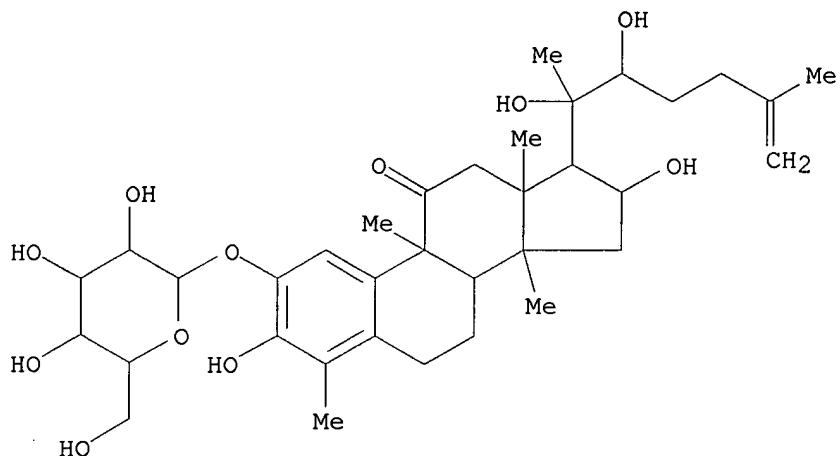
CN 19-Norcholesta-1,3,5(10),25-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 162857-59-2 HCAPLUS

CN 19-Norcholesta-1,3,5(10),25-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

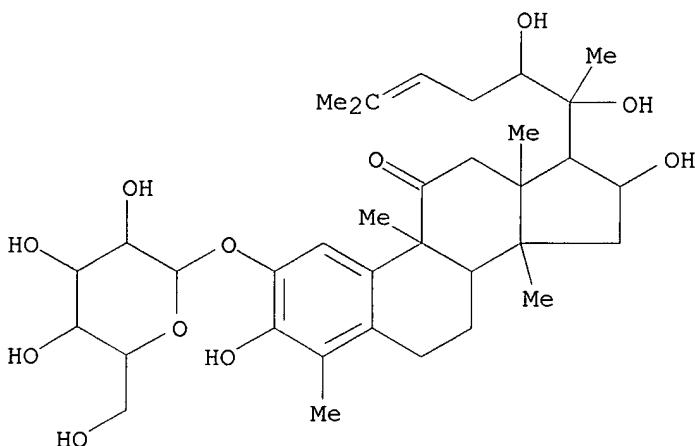
Currently available stereo shown.



RN 162857-60-5 HCAPLUS

CN 19-Norcholesta-1,3,5(10),24-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

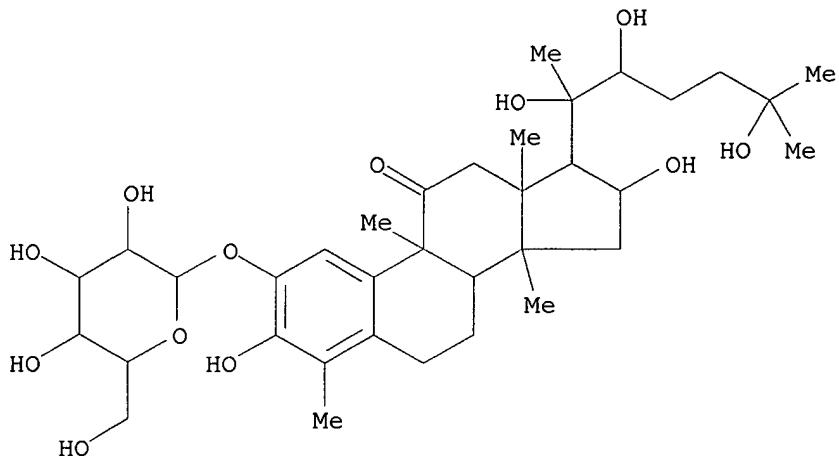
Currently available stereo shown.



RN 162857-61-6 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



L5 ANSWER 20 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:441021 HCAPLUS

DOCUMENT NUMBER: 122:286614

TITLE:

Studies on the constituents of the root of Cayaponia tayuya (Vell.) Cogn. I. Structures of cayaponosides, new 29-nor-1,2,3,4,5,10-hexadehydrocucurbitacin glucosides

AUTHOR(S):

Himeno, Eiji; Nagao, Tsuneatsu; Honda, Junko; Okabe, Hikaru; Irino, Nobuto; Nakasumi, Tetsuo

CORPORATE SOURCE:

Fac. Pharm. Sci., Fukuoka Univ., Fukuoka, 814-01, Japan

SOURCE:

Chemical & Pharmaceutical Bulletin (1994), 42(11), 2295-300

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER:

Pharmaceutical Society of Japan

DOCUMENT TYPE:

Journal

LANGUAGE: English

AB The bitter constituents in the root of Cayaponia tayuya (Vell.) Cogn. were investigated, and 24 29-norcucurbitacin glucosides, named cayaponosides, were isolated. Among them, the structures of cayaponosides A, A3, A4, A6, B, B2, B3, B4, C, C2, C5a, D and D1 were detd. based mainly on spectral analyses. They are all glucosides of 29-nor-1,2,3,4,5,10-hexadehydrocucurbitacins, different only in side chain structure.

IT 147742-04-9P, Cayaponoside A 147742-05-0P, Cayaponoside

B 147742-06-1P, Cayaponoside C 147764-94-1P,

Cayaponoside D 151589-19-4P, Cayaponoside C5a

151703-09-2P, Cayaponoside B4 151703-10-5P, Cayaponoside

C2 162857-56-9P, Cayaponoside A3 162857-57-0P,

Cayaponoside A4 162857-58-1P, Cayaponoside A6

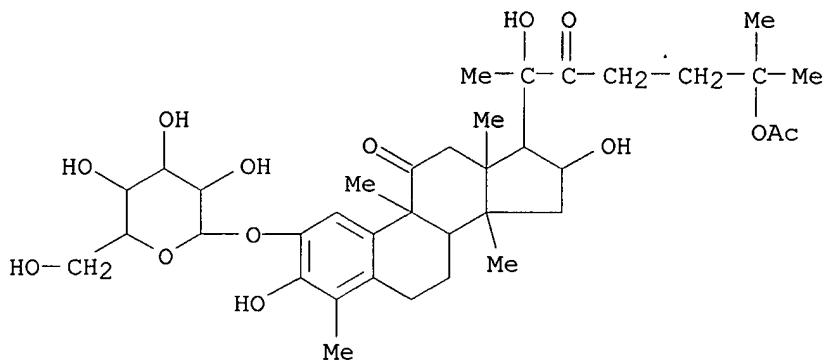
162857-59-2P, Cayaponoside B2 162857-60-5P, Cayaponoside

B3 162857-61-6P, Cayaponoside D1

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(from Cayaponia tayuya)

RN 147742-04-9 HCAPLUS

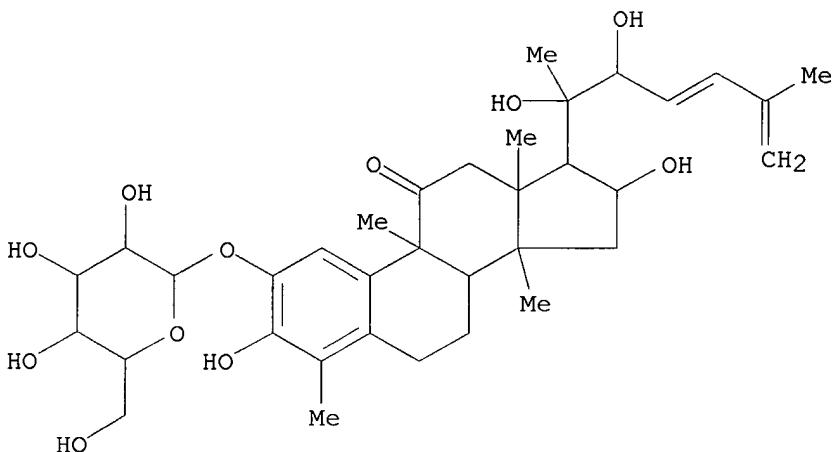
CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-(β-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-,

(9. β .,16. α .)- (9CI) (CA INDEX NAME)

RN 147742-05-0 HCPLUS

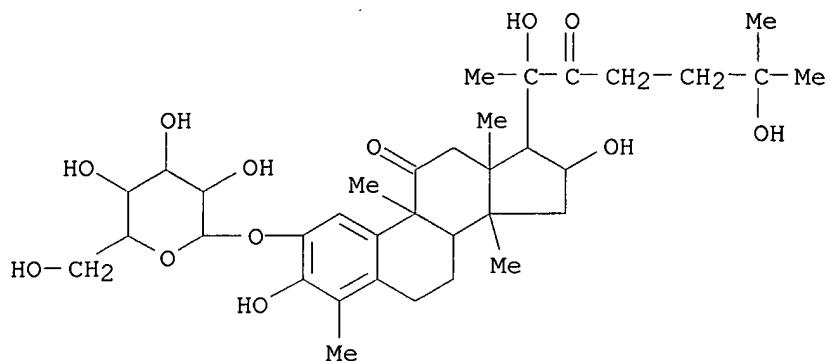
CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9. β .,16. α .)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 147742-06-1 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9. β .,16. α .)- (9CI) (CA INDEX NAME)



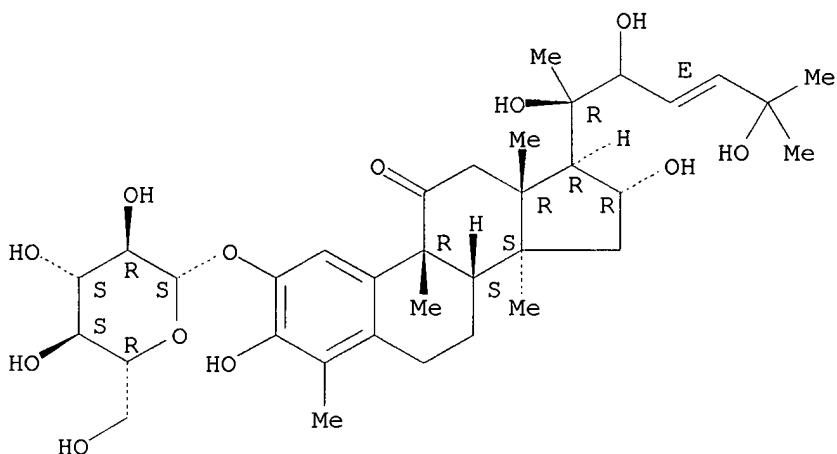
RN 147764-94-1 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Currently available stereo shown.

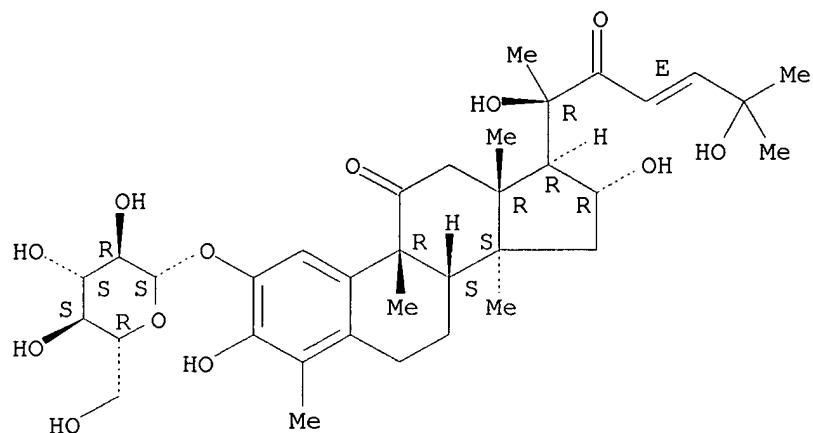


RN 151589-19-4 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

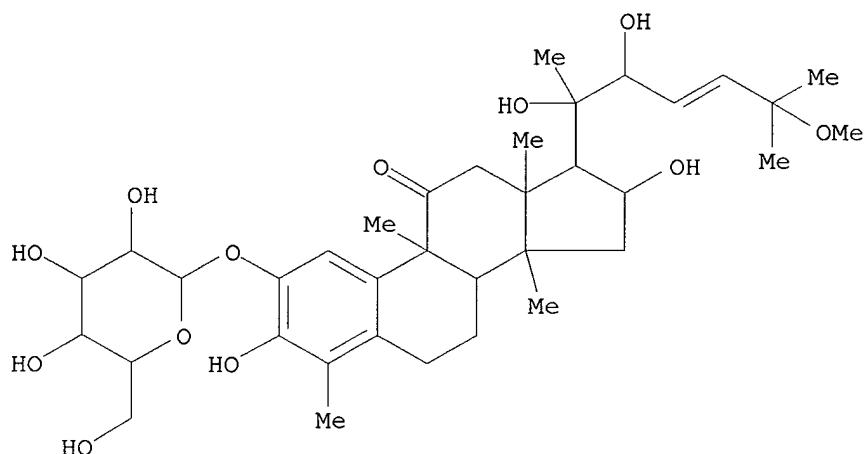
Double bond geometry as shown.



RN 151703-09-2 HCAPLUS

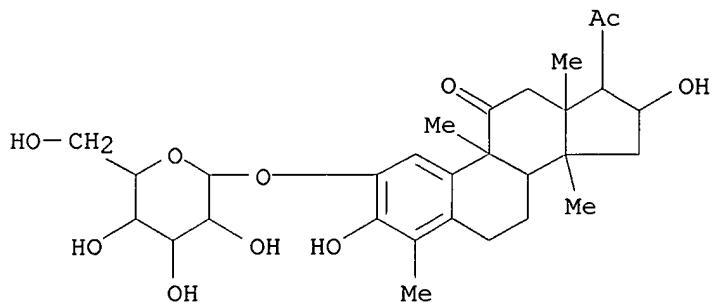
CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 151703-10-5 HCAPLUS

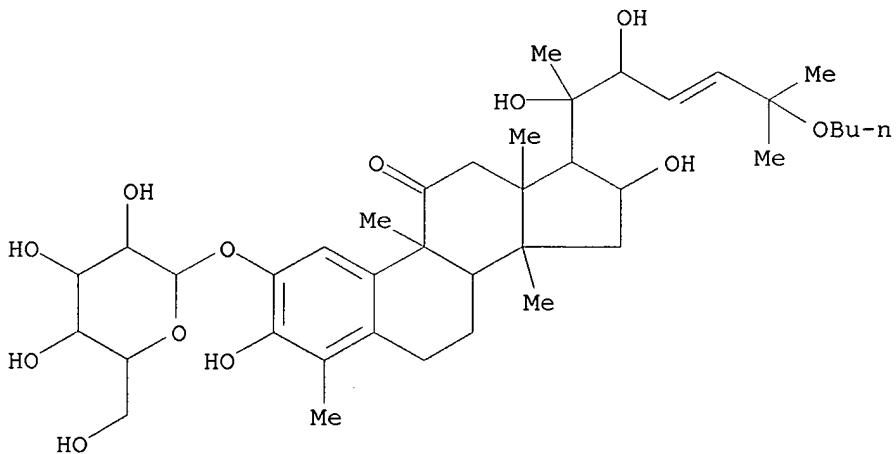
CN 19-Norpregna-1,3,5(10)-triene-11,20-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16-dihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 162857-56-9 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 25-butoxy-2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

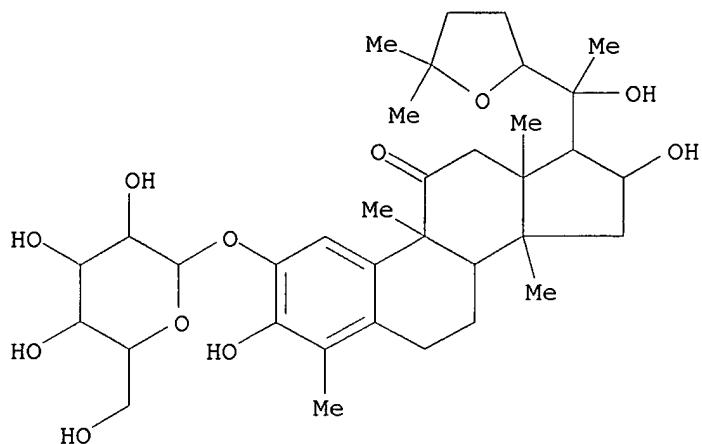
Currently available stereo shown.



RN 162857-57-0 HCPLUS

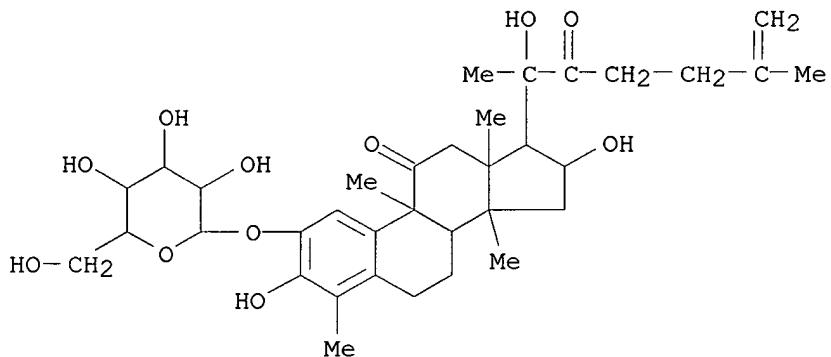
CN 19-Norcholesta-1,3,5(10)-trien-11-one, 22,25-epoxy-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 162857-58-1 HCPLUS

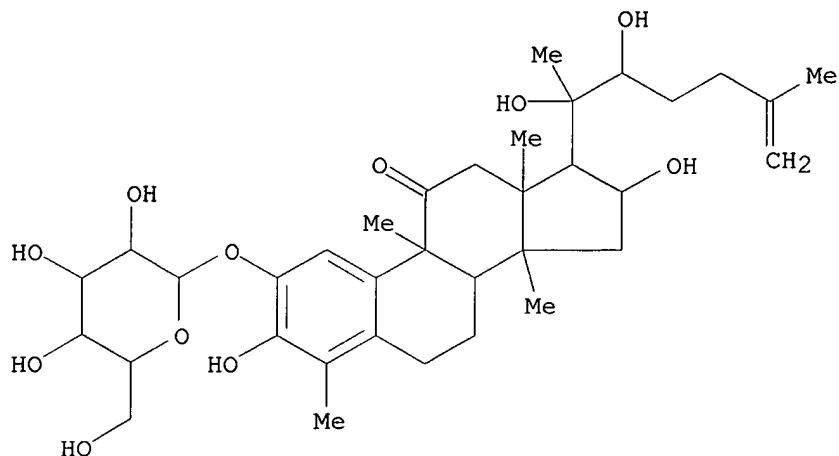
CN 19-Norcholesta-1,3,5(10),25-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 162857-59-2 HCPLUS

CN 19-Norcholesta-1,3,5(10),25-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

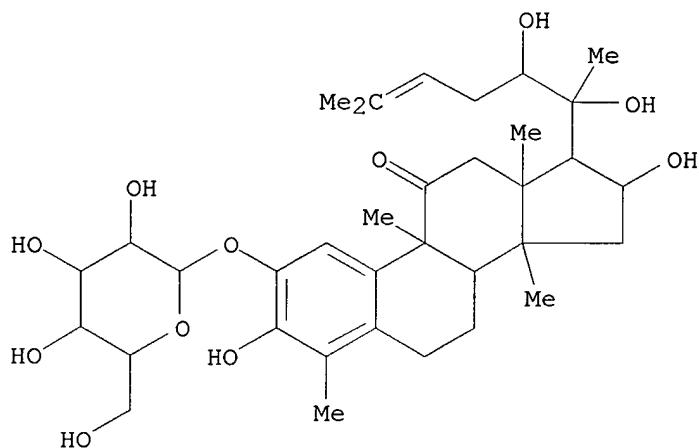
Currently available stereo shown.



RN 162857-60-5 HCPLUS

CN 19-Norcholesta-1,3,5(10),24-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

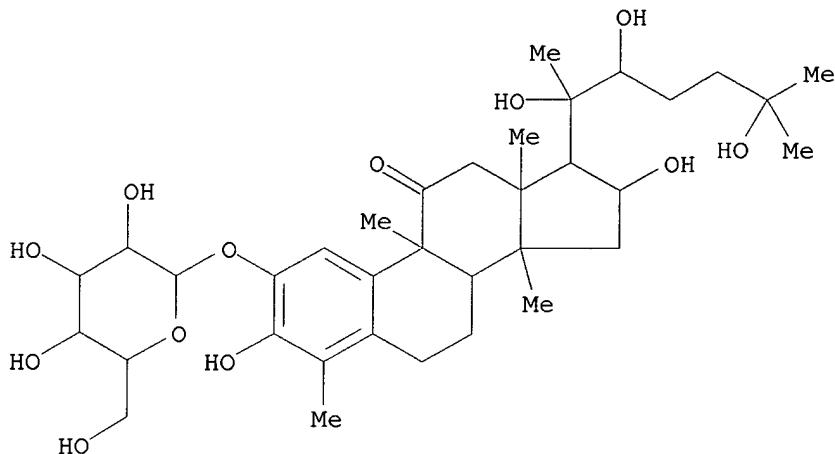
Currently available stereo shown.



RN 162857-61-6 HCPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



L5 ANSWER 21 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:276092 HCAPLUS

DOCUMENT NUMBER: 122:128588

TITLE: Norcucurbitacin gentiobiosides from Fevillea trilobata

AUTHOR(S): Valente, Ligia M. M.; Gunatilaka, A. A. Leslie;
Kingston, David G. I.; Pinto, Angelo C.

CORPORATE SOURCE: Department of Chemistry, Virginia Polytechnic
Institute and State University, Blacksburg, VA,
24061-0212, USA

SOURCE: Journal of Natural Products (1994), 57(11), 1560-3

CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The new norcucurbitacin glycosides, andirobin A gentiobioside (I), and andirobin C gentiobioside (II), and the known fevicordin F gentiobioside , were isolated from the aq. MeOH fraction of a liq.-liq. partition of the MeOH ext. of the seeds of Fevillea trilobata. Their structures were detd. by NMR and mass spectroscopy techniques.

IT 151589-26-3

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
BIOL (Biological study); OCCU (Occurrence)
(norcucurbitacin gentiobiosides from Fevillea trilobata)

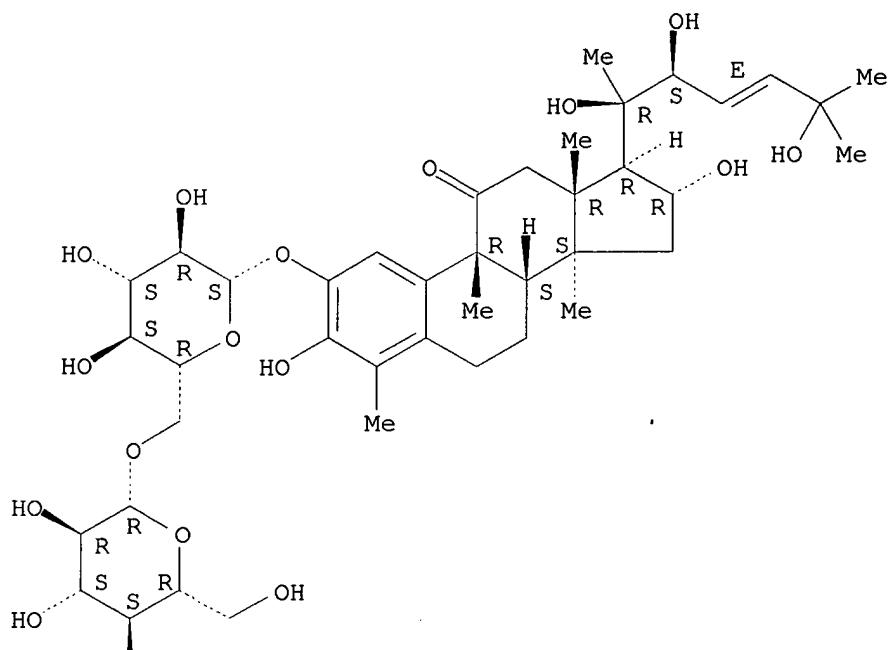
RN 151589-26-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

PAGE 1-A

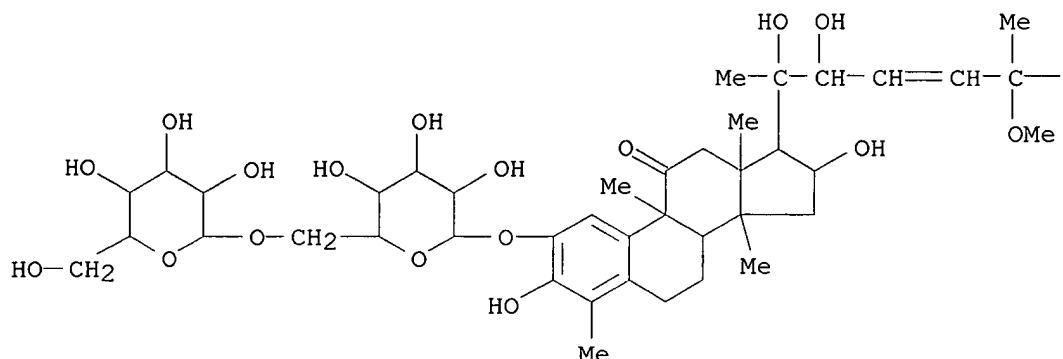


PAGE 2-A



- IT 161016-53-1P, Andirobin A 2-gentiobioside 161016-54-2P
, Andirobin C 2-gentiobioside
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(norcucurbitacin gentiobiosides from Fevillea trilobata)
- RN 161016-53-1 HCPLUS
- CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22-tetrahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

PAGE 1-A



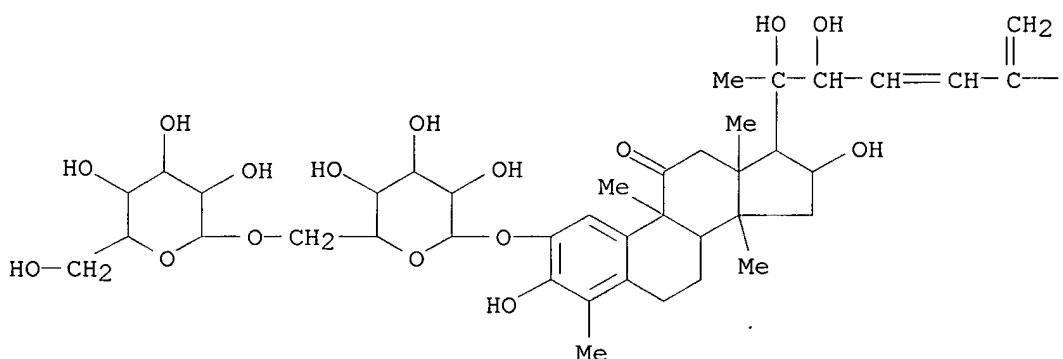
PAGE 1-B

— Me

RN 161016-54-2 HCPLUS

CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— Me

L5 ANSWER 22 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:261630 HCPLUS

DOCUMENT NUMBER: 120:261630

TITLE: Differentially regulated immediate early genes in the

AUTHOR(S):

rat uterus

CORPORATE SOURCE:

Bigsby, Robert M.; Li, Aixin
Sch. Med., Indiana Univ., Indianapolis, IN,
46202-5196, USA

SOURCE:

Endocrinology (1994), 134(4), 1820-6
CODEN: ENDOAO; ISSN: 0013-7227

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Estrogen stimulates cellular proliferation in the luminal epithelium, stroma, and smooth muscle of immature rat uterus. Progesterone administered concurrently with estrogen blocks the stimulatory effect of estrogen specifically in the epithelium, whereas progesterone administered alone stimulates proliferation in the endometrial stroma and myometrium. The present studies detd. the effects of estrogen and progesterone on expression of the growth-assocd., immediate early genes c-fos, c-jun, and jun-B in the luminal epithelium of the uterus. Hormonal effects were quantitated by Northern anal. of RNA extd. directly from the uterine luminal epithelium. Estrogen stimulated c-fos and jun-B expression, but repressed c-jun mRNA levels in the epithelium. In contrast, when whole organ RNA exts. were analyzed, estrogen increased mRNA levels for all three genes. Although progesterone administered alone showed no effect on mRNA levels in either epithelial or whole uterus exts., it did attenuate the estrogen-induced increase in c-fos mRNA by 50% in whole uterus exts. and by 23% in epithelial exts. The estrogen-induced increase in epithelial jun-B mRNA was not affected by progesterone pretreatment. Thus, in the immature rat uterus, no simple correlation exists between cellular proliferation and increased expression of the genes studied. However, progesterone completely blocked the repressive effect of estrogen on epithelial c-jun, suggesting a link between decreased c-jun expression and induction of cell proliferation in the uterine luminal epithelium. Estrogen repression of epithelial c-jun expression was hormone specific and sensitive to antiestrogen blockade. After estrogen treatment, epithelial c-jun mRNA decreased with a rate similar to its half-life, as detd. in primary cultures of rat uterine cells. These results suggest that estrogen, acting through its receptor, directly represses transcription of c-jun in the uterine epithelium. Differences in hormonal regulation of immediate early genes between epithelial and nonepithelial uterine tissues probably results from tissue-specific transactivating factors that control the expression of these genes.

IT 1090-04-6, 16.alpha.-Estradiol

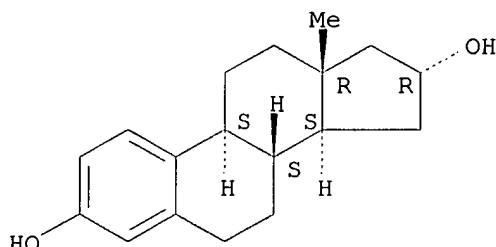
RL: BIOL (Biological study)

(immediate early gene expression in uterus response to)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 23 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1994:73386 HCPLUS
 DOCUMENT NUMBER: 120:73386
 TITLE: New nor- and hepta nor-cucurbitacin glucosides from Fevillea trilobata
 AUTHOR(S): Valente, Ligia M. M.; Gunatilaka, A. A. Leslie; Glass, Thomas E.; Kingston, David G. I.; Pinto, Angelo C.
 CORPORATE SOURCE: Dep. Chem., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061-0212, USA
 SOURCE: Journal of Natural Products (1993), 56(10), 1772-8
 CODEN: JNPRDF; ISSN: 0163-3864

DOCUMENT TYPE: Journal
 LANGUAGE: English

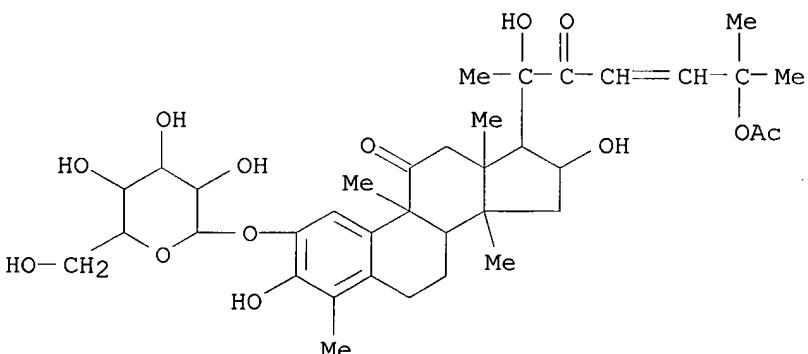
AB From the MeOH ext. of the seeds of Fevillea trilobata (Cucurbitaceae) were isolated fevicordin A glucoside (I), cayaponoside B, cayaponoside D, a new norcucurbitacin glucoside, and a new heptanorcucurbitacin glucoside. The structure of the new norcucurbitacin glucoside, andirobincin A glucoside (I), was established as 29-nor-1,2,3,4,5,10-dehydro-25-methoxy-2-O-.beta.-D-glucopyranosyl-3,16.alpha.,20R,22.xi.-tetrahydroxy-11-oxocucurbit-23-ene, and that of the novel heptanorcucurbitacin glucoside, andirobincin B glucoside, as 22,23,24,25,26,27,29-heptanor-1,2,3,4,5,10-dehydro-2-O-.beta.-D-glucopyranosyl-3,16.alpha.-dihydroxycucurbita-11,20-dione.

IT 111250-01-2, Fevicordin A glucoside 147742-05-0
 147764-94-1 152340-76-6D, Andirobincin B, derivs.
 152340-77-7D, Andirobincin A, derivs.

RL: BIOL (Biological study)
 (from Fevillea trilobata)

RN 111250-01-2 HCPLUS

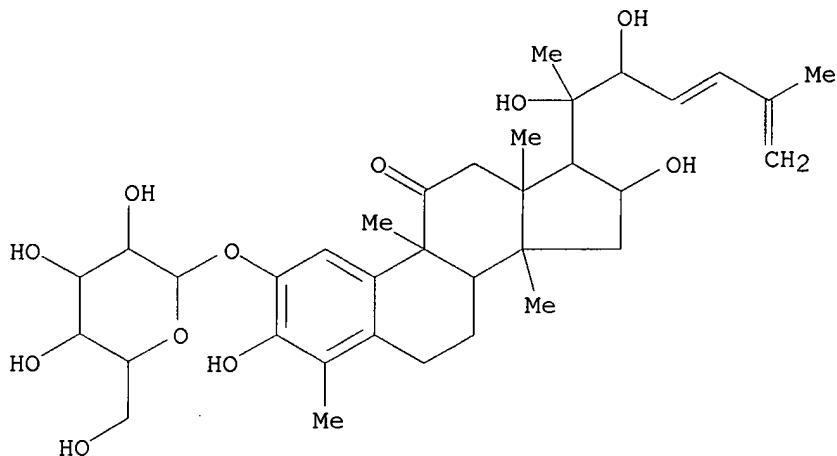
CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)



RN 147742-05-0 HCPLUS

CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-(β-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.β.,16.α.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



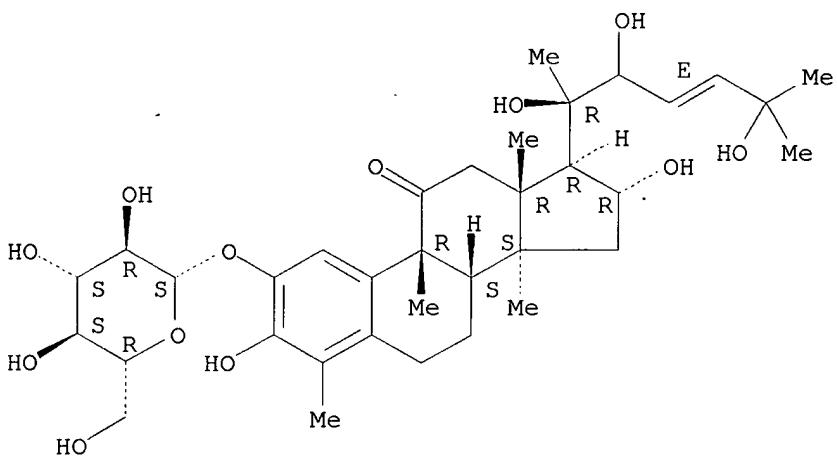
RN 147764-94-1 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

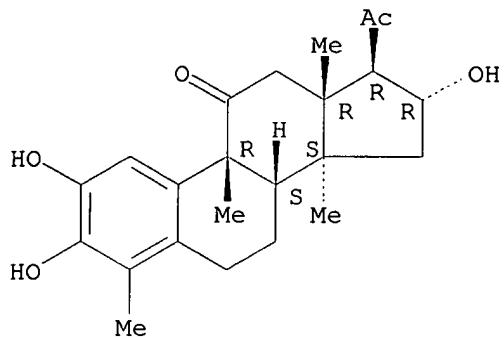
Currently available stereo shown.



RN 152340-76-6 HCPLUS

CN 19-Norpregna-1,3,5(10)-triene-11,20-dione, 2,3,16-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

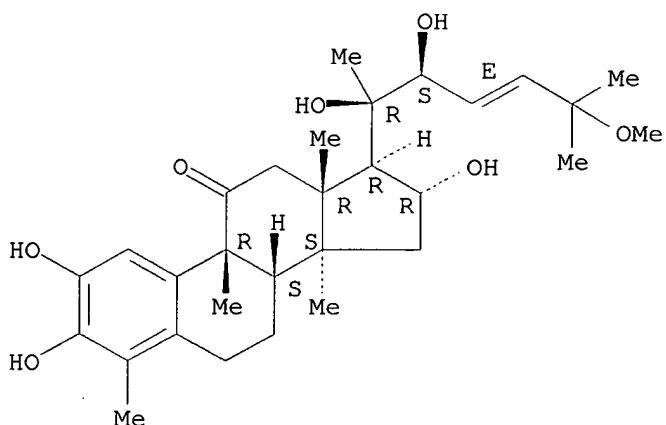


RN 152340-77-7 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,22-pentahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

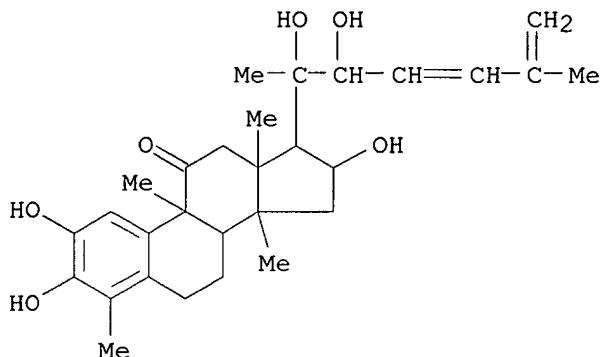


IT 151703-11-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 151703-11-6 HCPLUS

CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2,3,16,20,22-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



IT 151703-09-2 151703-10-5

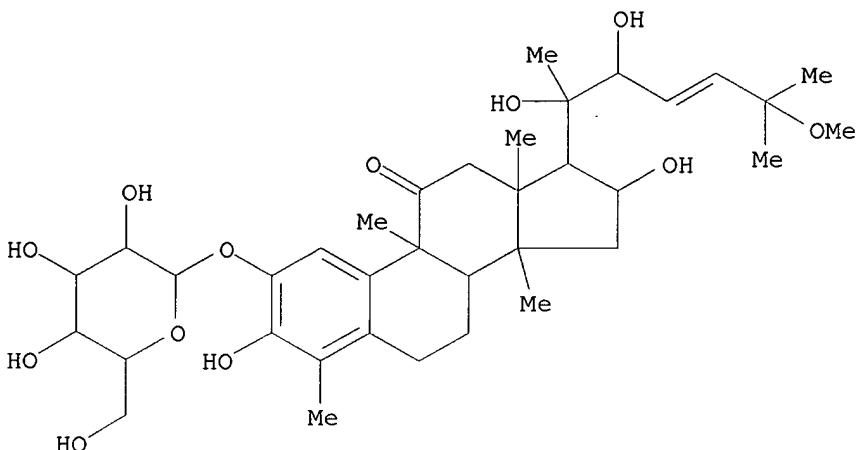
RL: PROC (Process)

(structure and isolation of, from Fevillea trilobata)

RN 151703-09-2 HCPLUS

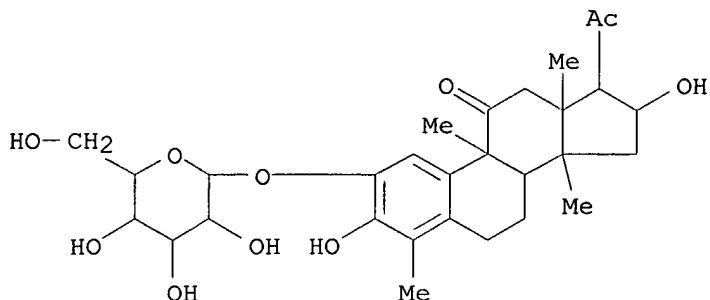
CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 151703-10-5 HCPLUS

CN 19-Norpregna-1,3,5(10)-triene-11,20-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16-dihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



L5 ANSWER 24 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:73357 HCAPLUS

DOCUMENT NUMBER: 120:73357

TITLE: Constituents of tropical medicinal plants. 59.

Constituents of Fevillea cordifolia: new
norcucurbitacin and cucurbitacin glycosidesAUTHOR(S): Achenbach, Hans; Waibel, Reiner; Hefter-Buebl, Ursula;
Constenla, Manuel A.CORPORATE SOURCE: Inst. Pharm. Food Chem., Univ. Erlangen, Erlangen,
D-91052, GermanySOURCE: Journal of Natural Products (1993), 56(9), 1506-19
CODEN: JNPRDF; ISSN: 0163-3864

DOCUMENT TYPE: Journal

LANGUAGE: English

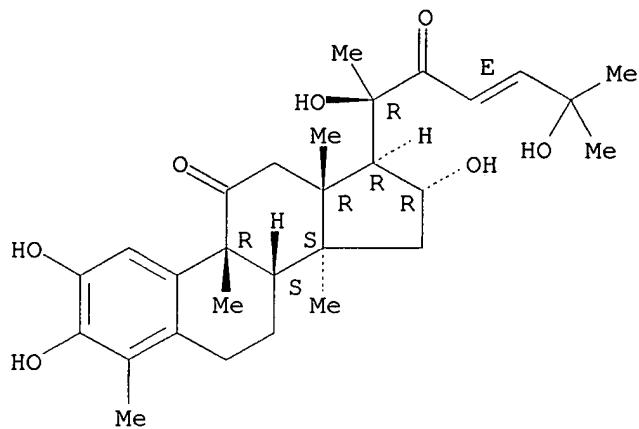
AB The seeds of *F. cordifolia* yielded 11 new fevicordin-type
29-norcucurbitacins and two new cucurbitacin glycosides, which were
isolated along with previous reported fevicordin A and its glucoside.
Structure detns. are based on spectroscopic studies and on chem.
interconversions.IT 152340-32-4D, Fevicordin C, derivs. 152340-33-5D,
Fevicordin D, derivs. 152340-34-6D, Fevicordin E, derivs.
152340-35-7D, Fevicordin F, derivs.RL: BIOL (Biological study)
(from *Fevillea cordifolia* seeds)

RN 152340-32-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2,3,16,20,25-
pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

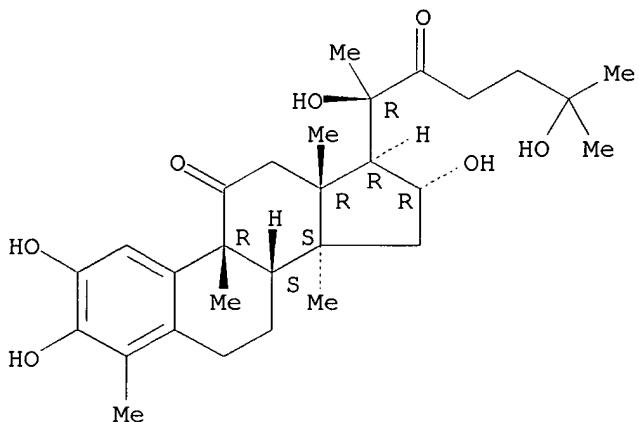
Double bond geometry as shown.



RN 152340-33-5 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

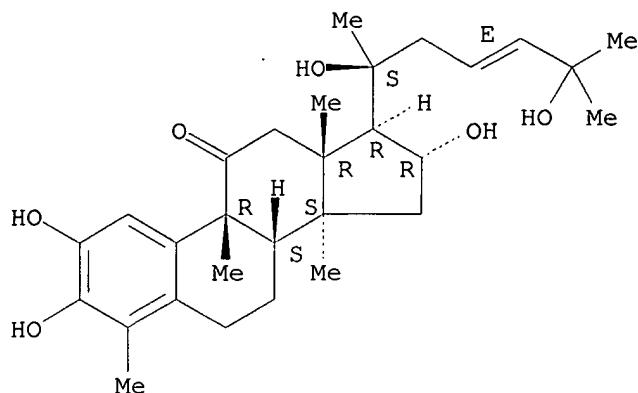


RN 152340-34-6 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

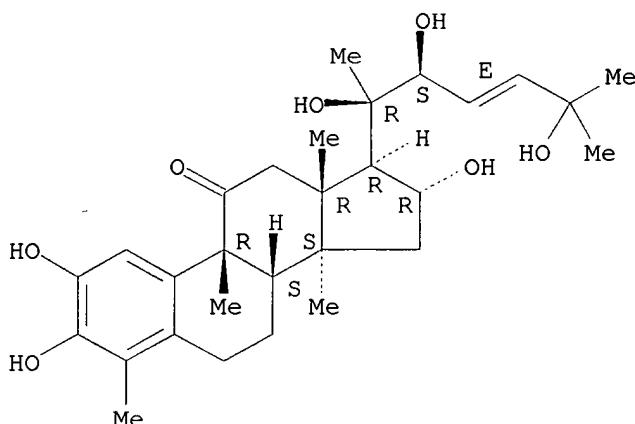


RN 152340-35-7 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,22,25-hexahydroxy-4,9,14-trimethyl-, (9. β .,16. α .,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 111250-01-2, Fevicordin A glucoside 111250-02-3,

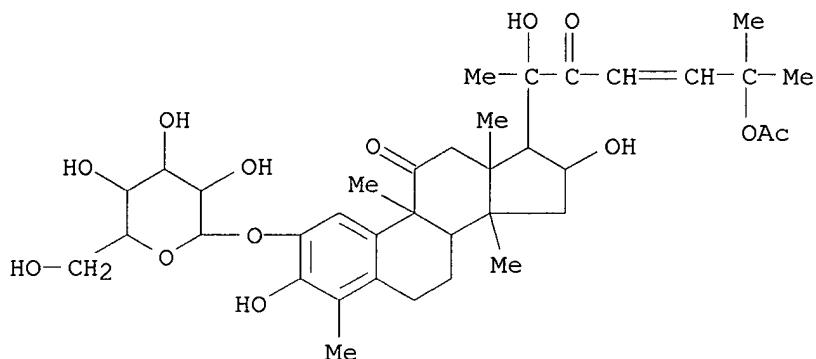
Fevicordin A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(from Fevillea cordifolia, antiinflammatory activity of)

RN 111250-01-2 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2-(β -D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9. β .,16. α .,23E)- (9CI) (CA INDEX NAME)

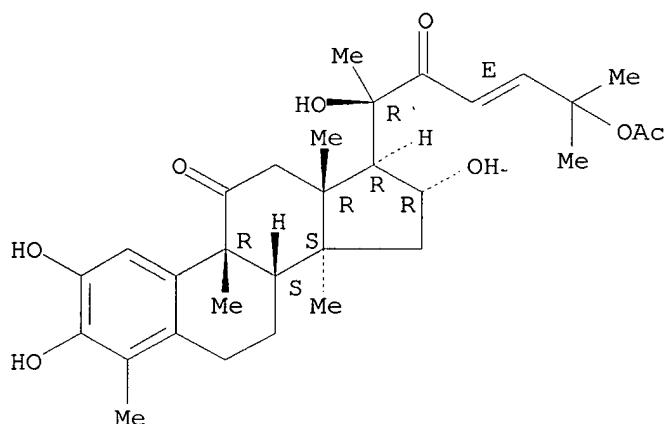


RN 111250-02-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9. beta., 16. alpha., 23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

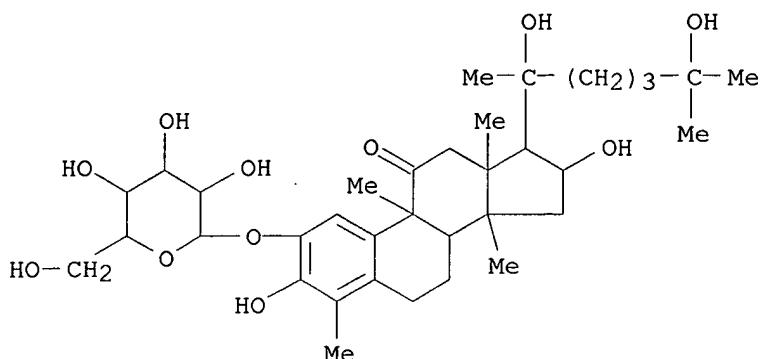


IT 151589-31-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of, by desoxygenation of fevicordin D glucoside)

RN 151589-31-0 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9. beta., 16. alpha.)- (9CI) (CA INDEX NAME)



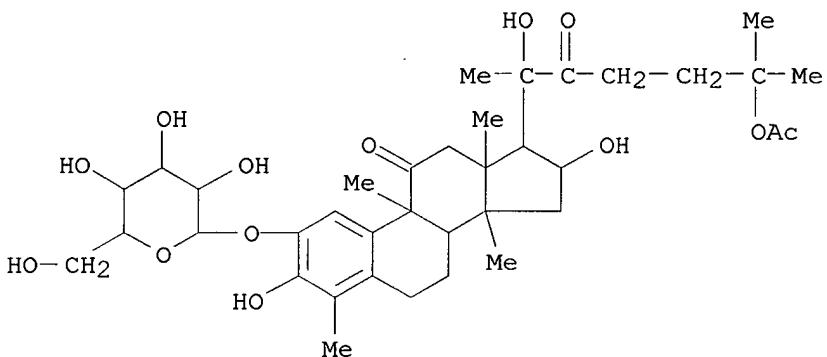
IT 147742-04-9 147742-06-1 151589-19-4
 151589-20-7 151589-21-8 151589-22-9
 151589-23-0 151589-24-1 151589-25-2
 151589-26-3 152340-09-5, Fevicordin B

RL: PROC (Process)

(structure and isolation of, from Fevillea cordifolia seeds)

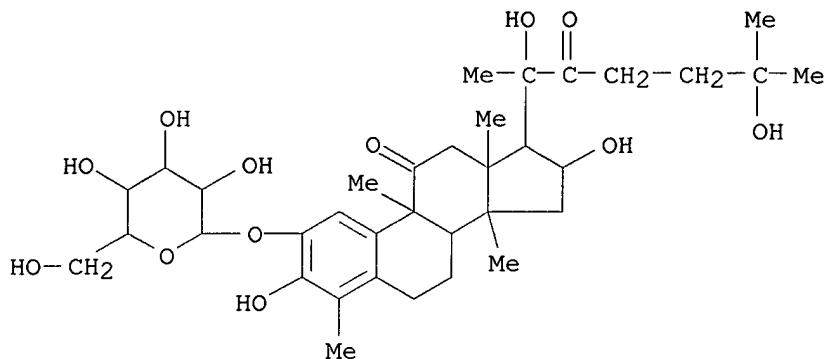
RN 147742-04-9 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetoxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-,
 (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 147742-06-1 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-,
 (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

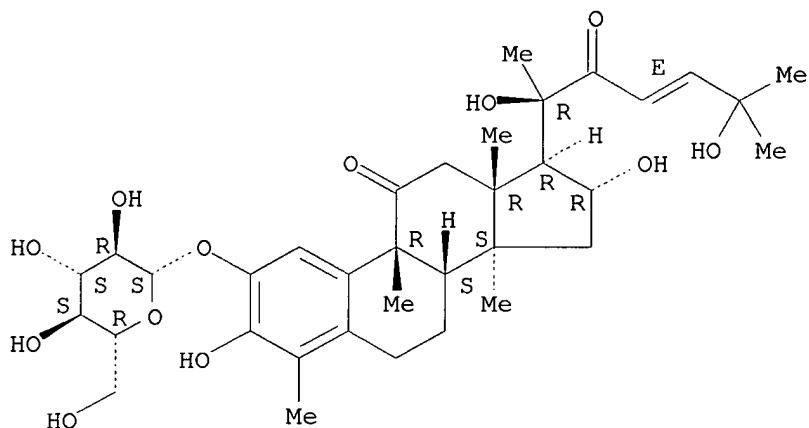


RN 151589-19-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

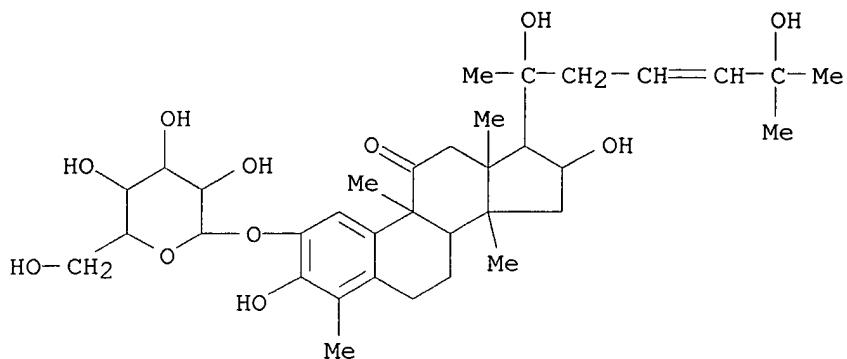
Absolute stereochemistry.

Double bond geometry as shown.



RN 151589-20-7 HCAPLUS

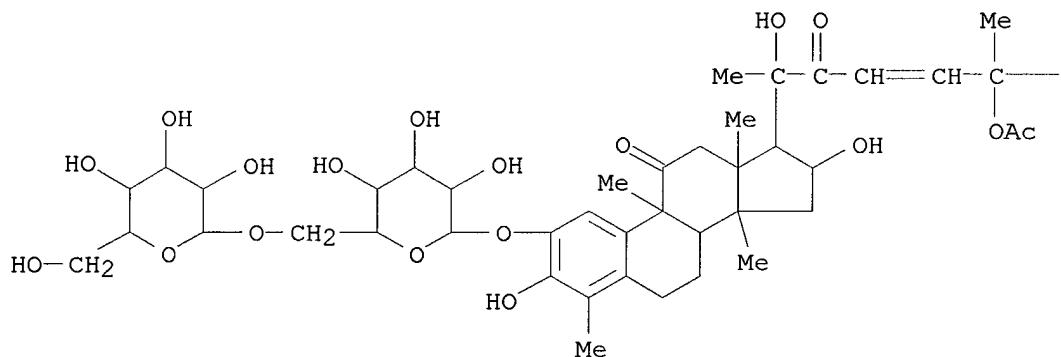
CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)



RN 151589-21-8 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

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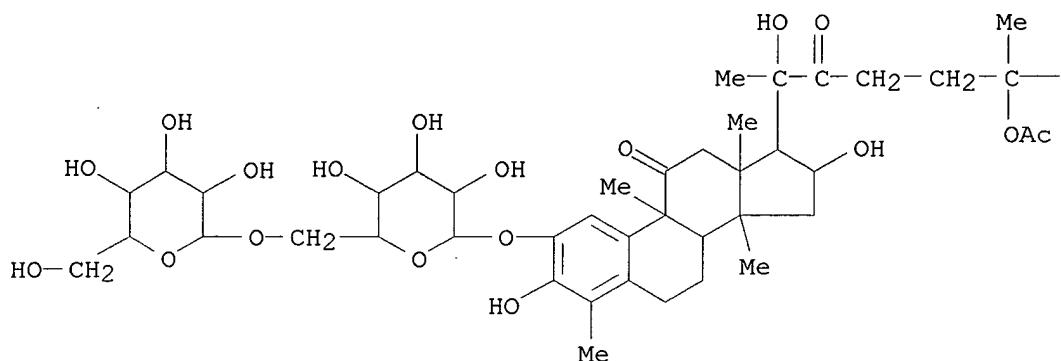
PAGE 1-B

— Me

RN 151589-22-9 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

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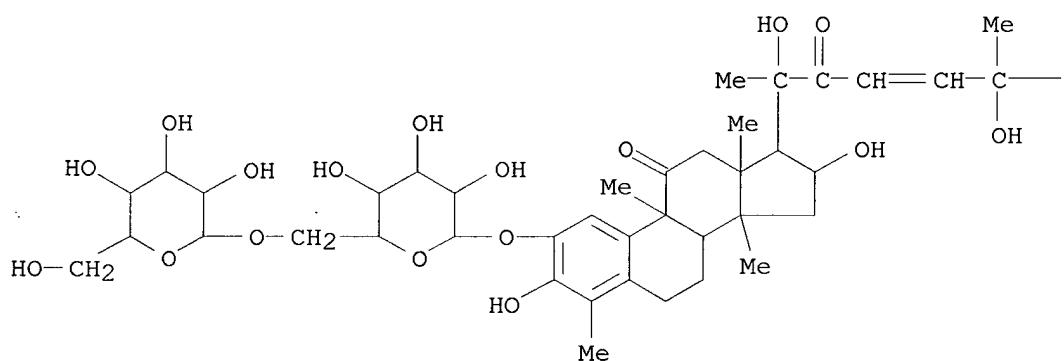
PAGE 1-B

— Me

RN 151589-23-0 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

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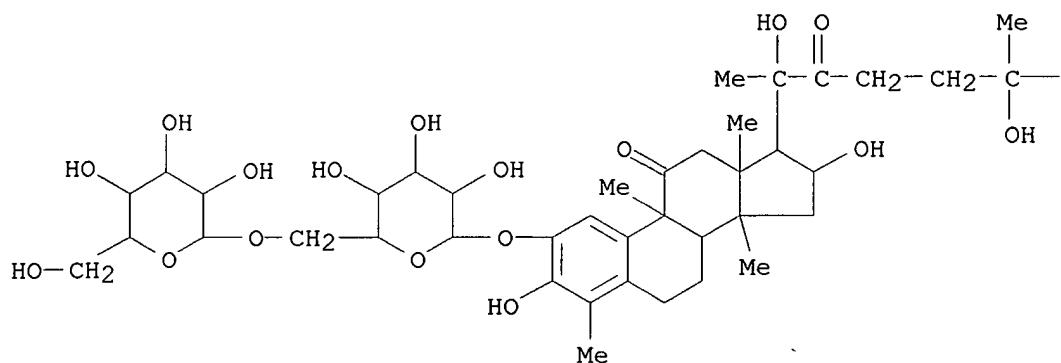
PAGE 1-B

— Me

RN 151589-24-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

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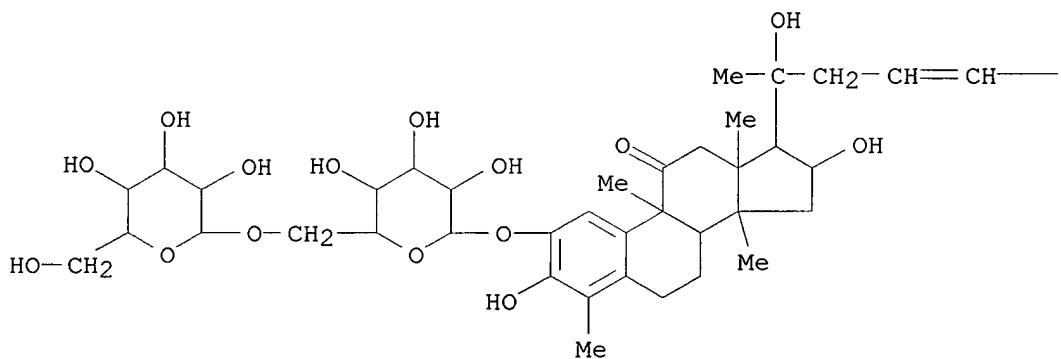
PAGE 1-B

— Me

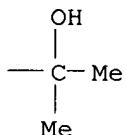
RN 151589-25-2 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

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PAGE 1-B



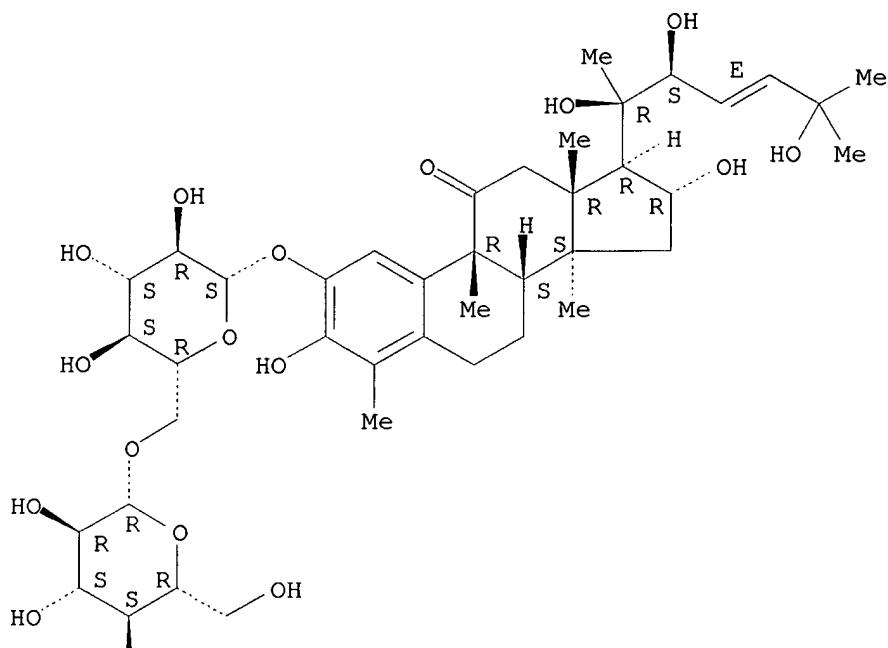
RN 151589-26-3 HCPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-[(6-O-.beta.-D-

glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22,25-pentahydroxy-
4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

PAGE 1-A

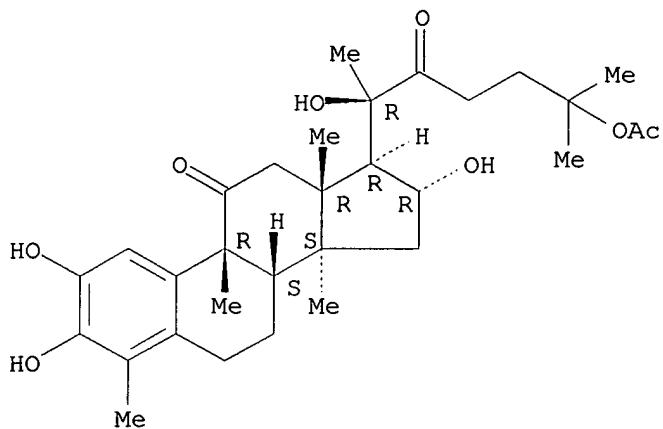


PAGE 2-A



RN 152340-09-5 HCAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 25 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:662769 HCAPLUS

DOCUMENT NUMBER: 119:262769

TITLE: Hormonal regulation and expression of the jun-D protooncogene in specific cell types of the rat uterus

AUTHOR(S): Nephew, Kenneth P.; Webb, David K.; Akcall, Kamil Can; Moulton, Bruce C.; Khan, Sohaib A.

CORPORATE SOURCE: Coll. Med., Univ. Cincinnati, Cincinnati, OH, 45267-0521, USA

SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1993), 46(3), 281-7

CODEN: JSBBEZ; ISSN: 0960-0760

DOCUMENT TYPE: Journal

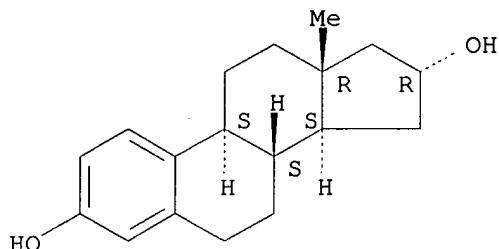
LANGUAGE: English

AB Steroid hormone regulation and cell-type specific expression of the jun-D protooncogene in rat uterus was exampd. Adult, ovariectomized rats were injected with progesterone, testosterone, 17.beta.-estradiol (E2-17.beta.), 16.alpha.-estradiol (E2-16.alpha.), dexamethasone or cycloheximide. Uteri were collected between 0 and 6 h post-treatment. Northern blot anal. of uterine RNA revealed that induction of jun-D was specific for estrogenic steroids, as progesterone and testosterone had no effect on expression of this member of the jun gene family. Treatment with E2-17.beta. increased jun-D mRNA levels by approx. 5-fold, with expression reaching peak levels at 3 h after treatment and declining thereafter. Administration of E2-16.alpha., a short-acting estrogen that does not cause uterine cell proliferation, increased expression of jun-D but with different kinetics than that of the long-acting E2-17.beta.. The mRNA levels of jun-D increased by 3-fold 1 h after administration of E2-16.alpha. but declined soon after. Slight induction of jun-D mRNA by dexamethasone was apparent, but to a much lesser extent compared to estrogen. The protein synthesis inhibitor, cycloheximide, did not block jun-D induction, indicating that this is an immediate early response. Expression of Jun-D protein was exampd. by immunohistochem. methods. E2-17.beta. treatment activated jun-D primarily in the nuclei of luminal and glandular epithelial cells of the endometrium. These results demonstrate that hormonal induction of jun-D is specific for estrogens and that uterine expression of this protooncogene occurs in a cell-type specific manner.

IT 1090-04-6, 16.alpha.-Estradiol

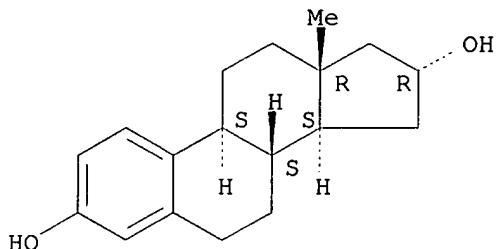
RL: BIOL (Biological study)
 (jun-D expression in uterus response to)
 RN 1090-04-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 26 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1993:552319 HCAPLUS
 DOCUMENT NUMBER: 119:152319
 TITLE: Estrogen induces expression of c-jun and jun-B protooncogenes in specific rat uterine cells
 AUTHOR(S): Webb, David K.; Moulton, Bruce C.; Khan, Sohaib A.
 CORPORATE SOURCE: Coll. Med., Univ. Cincinnati, Cincinnati, OH,
 45267-0521, USA
 SOURCE: Endocrinology (1993), 133(1), 20-8
 CODEN: ENDOAO; ISSN: 0013-7227
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Expression of the protooncogene c-jun is induced in the uteri of ovariectomized rats in response to treatment with 17.beta.-estradiol (E2). E2 also specifically induces the uterine expression of jun-B-encoding mRNA. Medroxyprogesterone acetate and testosterone propionate treatment had no effect on the expression of c-jun- and jun-B-encoding mRNAs. Dexamethasone treatment, however, induced expression of c-jun mRNA, although less than that obsd. in response to E2. Cycloheximide treatment failed to block the E2-induced expression of c-jun and jun-B mRNAs, indicating that these were immediate early responses. 16.alpha.-Estradiol, a short-acting estrogen, also induced c-jun and jun-B mRNA expression. The expression of c-Jun protein was exampd. by immunohistol. methods and detected in all uterine cell types in response to treatment with estrogen. The Jun-B protein, however, was localized in uterine epithelial cells. The results of these expts. suggest that the cell type-specific expression of members of the jun family of protooncogenes may be an important regulatory event in the response of the uterus to estrogen.
 IT 1090-04-6
 RL: BIOL (Biological study)
 (gene c-jun and gene jun-B expression induction by, in uterus)
 RN 1090-04-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 27 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:531757 HCAPLUS

DOCUMENT NUMBER: 119:131757

TITLE: Influence of estrogen structure on nuclear binding and progesterone receptor induction by the receptor complex

AUTHOR(S): VanderKuur, J. A.; Wiese, T.; Brooks, S. C.

CORPORATE SOURCE: Sch. Med., Wayne State Univ., Detroit, MI, 48201, USA

SOURCE: Biochemistry (1993), 32(27), 7002-8

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The relationship between steroid structure, estrogen receptor (ER) binding affinity, nuclear binding of the ER complex, and induction of progesterone receptor (PgR) have been examd. The level of ER in membrane-free homogenates of MCF-7 cells was 10.0 fmol/.mu.g of DNA as detd. by an EIA. However, only 2.5 fmol of ER complex/.mu.g of DNA was bound by nuclei during maximal stimulation of PgR synthesis (2.9 fmol of PgR/.mu.g of DNA; measured by EIA) following a pulse with 10-10 M E2. Except at micromolar concns., estratriene was an ineffective estrogen. The addn. of a hydroxyl group to either position 3 or position 17.beta. of estratriene yielded ligands which were capable of causing nuclear binding and processing of ER as well as PgR induction. D-ring regioisomers of estradiol (E2) had lower affinity for receptor than E2. However, receptor complexed with these estrogens was fully capable of binding to nuclear material, undergoing processing, and inducing PgR. On the other hand, A-ring regioisomers of E2 displayed differences in their ability to mediate nuclear binding of receptor complex and induction of PgR. Although 1-hydroxyestratrien-17.beta.-ol was weakly bound by ER, this dihydroxyestrogen was capable of bringing about nuclear binding and processing of ER and the stimulation of PgR synthesis. In contrast, 2- and 4-hydroxyestratrien-17.beta.-ol, which caused extensive nuclear binding of ER 95-7 fmol/.mu.g of DNA), were incapable of PgR induction. Provided that the A-ring hydroxyl group was positioned correctly (3.beta.) on androstanediols, an arom. ring was not required for nuclear binding of the ER complex and stimulation of PgR synthesis. With the except of 2- and 4-hydroxyestratrien-17.beta.-ol, induction of PgR by structurally altered estrogens correlated with the affinity of ligand for ER. Electrostatic models generated from this data were found to be useful in the characterization of electroneg. isopotential regions of the estrogen (or androstandiol) mols. which were important in modulating the gene regulatory properties of ER.

IT 1090-04-6, 16.alpha.-Estradiol

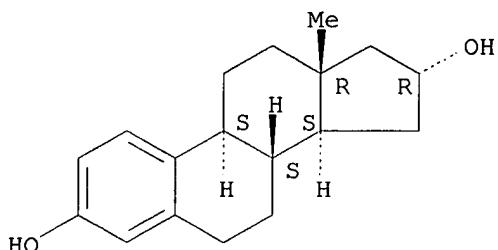
RL: BIOL (Biological study)

(estrogen receptor complex binding by nucleus and progesterone receptor induction by, in MCF-7 cells, mol. structure in relation to)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 28 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:441184 HCAPLUS

DOCUMENT NUMBER: 119:41184

TITLE: Differential induction of pS2 and cathepsin D mRNAs by structurally altered estrogens

AUTHOR(S): Pilat, M. J.; Hafner, M. S.; Kral, L. G.; Brooks, S. C.

CORPORATE SOURCE: Sch. Med., Wayne State Univ., Detroit, MI, 48201, USA

SOURCE: Biochemistry (1993), 32(27), 7009-15

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The influence of structural alterations to the estradiol (E2) mol. on the induction of pS2 and cathepsin D (Cath D) mRNAs has been examd. by Northern anal. of RNA extd. from MCF-7 cells. Exposure of cultures to estratriene did not affect the level of expression of these estrogen-responsive genes. Addn. of one hydroxyl group to estratriene at either of the hydroxylated positions of E2 (3-phenolic or 17.beta.) yielded monohydroxyestrogens which stimulated the synthesis of Cath D and pS2 mRNAs to a level comparable to that induced by 10-10 M E2 and displayed a decrease in activity at the higher concns. (10⁻⁸-10⁻⁷ M) similar to that of the parent estrogen. Both of these genes were induced maximally by estrogens with D-ring alterations. Movement of the phenolic hydroxyl group of E2 to other positions on the A-ring yielded ligands which were highly discriminatory in the induction of these messages. 1-Hydroxyestratrien-17.beta.-ol was capable of stimulating maximal synthesis of both pS2 and Cath D mRNAs when added to cultures of MCF-7 cells at a concn. of 10⁻⁸ M. Placement of the phenolic hydroxyl at position 4 greatly diminished the induction of these 2 estrogen-responsive genes. On the other hand, positioning the A-ring hydroxyl group on carbon 2 yielded a ligand which brought about the induction of one gene (pS2) but was marginally effective in the induction of Cath D mRNA synthesis. 5.alpha.-Androstanediol and 5-androstenediol, with 17.beta.-hydroxyl, were both capable of inducing both genes, provided the 3-hydroxyl group was in the .beta.-configuration. Thus, discrete changes in the structure of estradiol generate ligands (2- or 4-hydroxyestradien-17.beta.-ol) with affinities for the estrogen receptor which are not related to their capacity to regulate certain responsive genes (pS2 or Cath D). It is proposed that the obsd. discrimination between these 2 responsive genes is the result of variations in the receptor-analog complex which are

important in interactions with gene regulatory favors (e.g., estrogen response element and/or transactivation function 2). Furthermore, the spatial placement of the electroneg. isopotential surrounding the arom. A-ring of these estrogen analogs appears to be involved in the modulation of gene regulation.

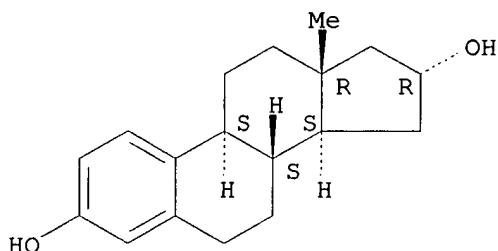
IT 1090-04-6

RL: BIOL (Biological study)
(cathepsin D and gene pS2 mRNAs induction by, in MDCF-7 cells, mol.
structure in relation to)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 29 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:441183 HCAPLUS

DOCUMENT NUMBER: 119:41183

TITLE: Effects of 17.beta.-estradiol analogs on activation of estrogen response element regulated chloramphenicol acetyltransferase expression

AUTHOR(S): VanderKuur, J. A.; Hafner, M. S.; Christman, J. K.; Brooks, S. C.

CORPORATE SOURCE: Sch. Med., Wayne State Univ., Detroit, MI, 48201, USA

SOURCE: Biochemistry (1993), 32(27), 7016-21

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB These expts. were designed to examine the effect of structural modifications to the 17.beta.-estradiol (E2) mol. on the estrogen response element (ERE)-dependent activation of the thymidine kinase (tk) promoter. Estrogen receptor (ER)-pos. MCF-7 cells were transfected with plasmids contg. 1 or 2 vitellogenin EREs inserted 39-53 nucleotides upstream of the tk promoter in p(-37)tk. Transient expression of the CAT gene in these constructs was measured after cells had been maintained for 36-42 h in the presence of E2 or an E2 analog. E2 induced CAT expression at levels as low as 10-13M, with max. induction at 10-11M. CAT activity decreased at higher concns. of E2. Estratriene, which has low affinity for ER, was active only at micromolar concns. 3-Hydroxyestratriene displayed maximal activity at 10-9M, with higher levels being less active. Still higher concns. (10-7M) of estratrien-17.beta.-ol were required to induce max. CAT activity. All positional and conformational alterations in the D-ring hydroxyl group of E2 yielded active ligands. Movement of the phenolic hydroxyl group of E2 to other positions on the A-ring produced dihydroxyestrogens with varied capacities to activate CAT (2-hydroxyestratrien-17.beta.-ol produced max. CAT activation at 10-11M;

1-hydroxyestratrien-17.beta.-ol required a 10-8M concn. for max. activity; 4-hydroxyestratrien-17-.beta.-ol gave max. CAT activation at 10-6M). Only those androstanediols or 5-androstenediols with a 3.beta.-hydroxyl group were capable of activating CAT expression. CAT constructs with 2 consensus EREs placed 6 or 19 bp apart were equally active and displayed a response to E2 or to the estrogen analogs similar to that of plasmids with a single consensus ERE. The concns. of structurally modified estrogens which generated max. CAT responses from these constructs were directly related to their affinity for ER. This contrasts with results obtained with the more complex regulatory regions of endogenous E2-responsive genes in MCF-7 cells. It is suggested that transcriptional activation following the binding of ER-ligand complexes to the ERE can be modulated by interactions with factors bound to other cis regulatory elements. Such protein-protein interactions appear to be influenced by the structure of the ligand.

IT 1090-04-6, 16.alpha.-Estradiol

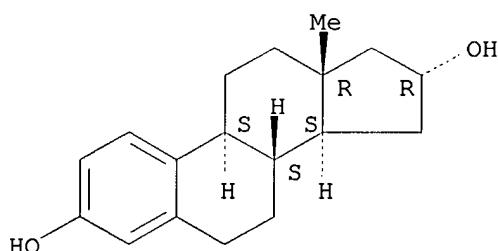
RL: PRP (Properties)

(estrogen response element-regulated cloramphenicol acetyltransferase expression induction by, mol. structure in relation to)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 30 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:251420 HCAPLUS

DOCUMENT NUMBER: 118:251420

TITLE: Structures of cayaponosides A, B, C and D, glucosides of new nor-cucurbitacins in the roots of Cayaponia tayuya

AUTHOR(S): Himeno, Eiji; Nagao, Tsuneatsu; Honda, Junko; Okabe, Hikaru; Irino, Nobuto; Nakasumi, Tetsuo

CORPORATE SOURCE: Fac. Pharm. Sci., Fukuoka Univ., Fukuoka, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1992), 40(10), 2885-7

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Four glucosides of new nor-cucurbitacins having an aromatized A ring were isolated from the roots of Cayaponia tayuya. Their structures of these bitter compds. were elucidated by spectral methods to be: cayaponoside A (I), cayaponoside B (II), cayaponoside C (III), and cayaponoside D (IV).

IT 147742-04-9, Cayaponoside A 147742-05-0, Cayaponoside B

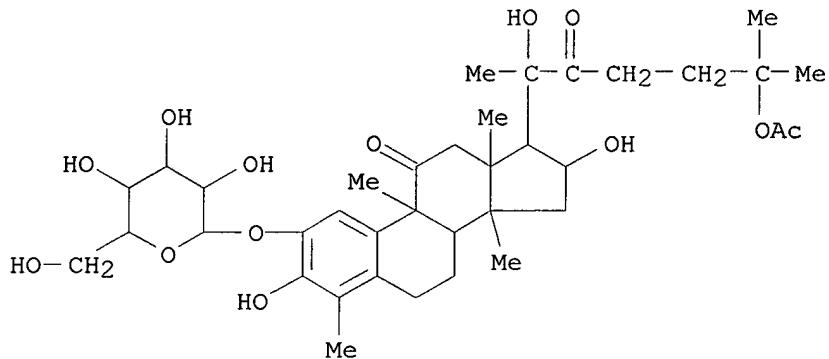
147742-06-1, Cayaponoside C 147764-94-1, Cayaponoside D

RL: PROC (Process)

(structure and isolation of, from Cayaponia tayuya roots, bitterness in relation to)

RN 147742-04-9 HCPLUS

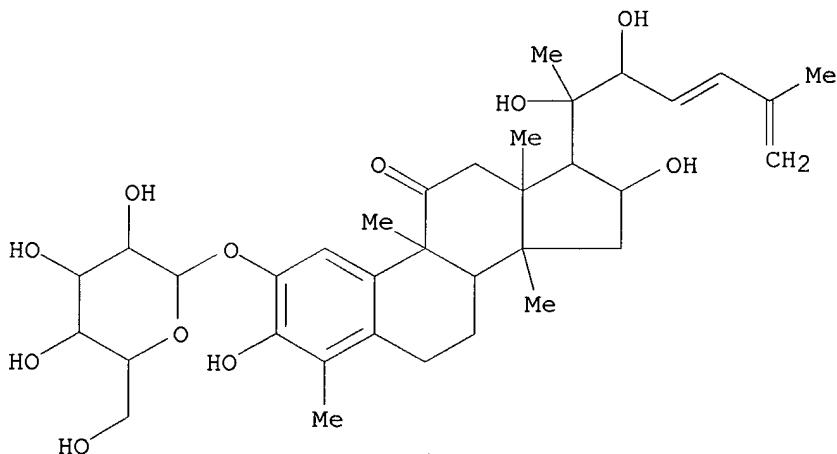
CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 147742-05-0 HCPLUS

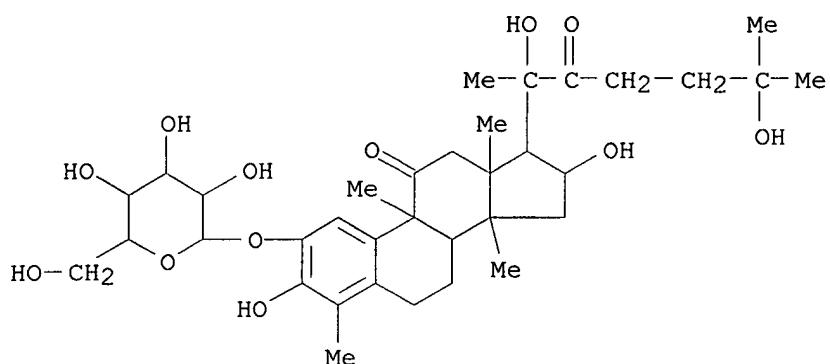
CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 147742-06-1 HCPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



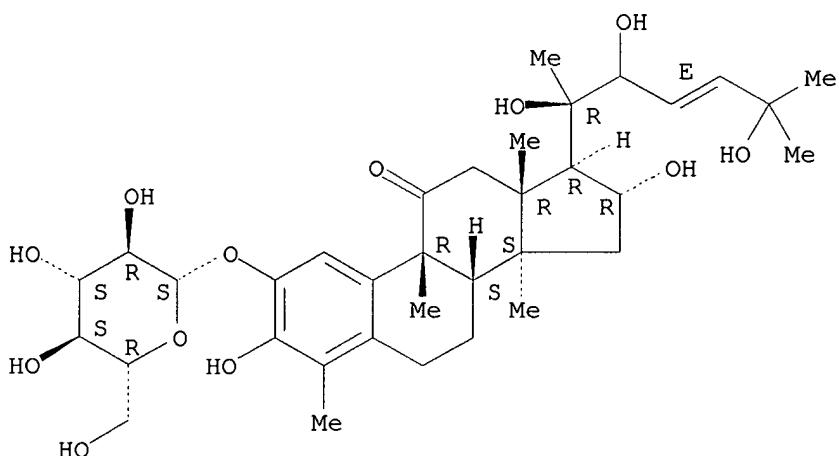
RN 147764-94-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Currently available stereo shown.



L5 ANSWER 31 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:506445 HCAPLUS

DOCUMENT NUMBER: 115:106445

TITLE: Uterine estrogen receptor-DNA complexes: effects of different ERE sequences, ligands, and receptor forms

AUTHOR(S): Curtis, Sylvia W.; Korach, Kenneth S.

CORPORATE SOURCE: Lab. Reprod. Dev. Toxicol., Natl. Inst. Environ.

Health Sci., Research Triangle Park, NC, 27709, USA

SOURCE: Molecular Endocrinology (1991), 5(7), 959-66

CODEN: MOENEN; ISSN: 0888-8809

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previous studies used the gel retardation assay to examine the binding of the mouse estrogen receptor (ER) to the estrogen-responsive element (ERE)

from the vitellogenin A2 gene (VitA2ERE). Multiple specific complexes were formed when the ER was bound to various estrogen agonists or antagonists, or in the absence of bound hormone. The ERE from the human PS2 gene, which varies from the consensus ERE by one base change in the right arm, was used in this study to det. the effect of DNA sequence on ER-ERE interaction with various ligand-receptor complexes. Partially purified ligand-free sol. ER showed a 3-fold lower affinity for the PS2ERE than for the VitA2ERE, suggesting a possible influence of the imperfect DNA sequence on certain binding interactions. However, multiple complexes of similar affinity were formed with the PS2 sequence by nuclear ER regardless of the agonist or antagonist bound. In gel retardation expts., antagonist (LY117018) nuclear ER complexes bound to either PS2 or VitA2ERE migrated more slowly than agonist complexes, indicating that the slower migrating form of the complex was not due to the DNA sequence. Interestingly, sol. ER bound by LY 117018 did not produce this decreased mobility complex, suggesting that it was specific to the nuclear form of the ER antagonist complex. Receptor activation has been linked with exposure to increased temp., resulting in an ER form that has an increased affinity for DNA. The binding of molybdate-stabilized nonactivated 8S ER to VitA2ERE was studied to det. the effect of temp. on ER binding. Heat pretreatment of the stabilized sol. 8S ER did not cause an increase in ER-ERE binding during a 45-min reaction. Heat pretreatment slightly increased the final level of complex formed when followed for 24 h, but this temp. activation of the ER is also simply a reflection of an increased reaction rate of the complex formation between the ER and the ERE. Molybdate-stabilized sol. ER formed two specific ERE complexes. Partial purifn. of the stabilized sol. ER resulted in formation of only one specific ERE complex. This differential multiplicity of ER-ERE complexes formed with native ER exts. may be due to the presence of addnl. factors which contribute to the formation of the complexes. Studies are presently underway to identify these factors from uterine tissue. This study, using various uterine ER forms and different ERE sequences, suggests that the effect of estrogen on gene expression is not mediated only at the level of ER-ERE interaction, but may occur through regulation of ER interaction with addnl. nuclear structures or proteins involved in transcription.

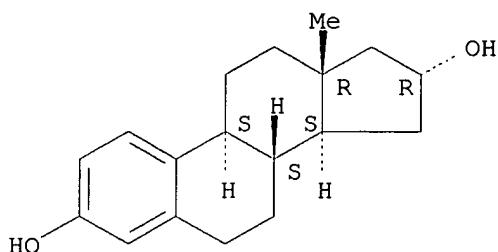
IT 1090-04-6D, 16.alpha.-Estradiol, receptor complexes

RL: BIOL (Biological study)
(ERE binding by, of uterus)

RN 1090-04-6 HCAPLUS

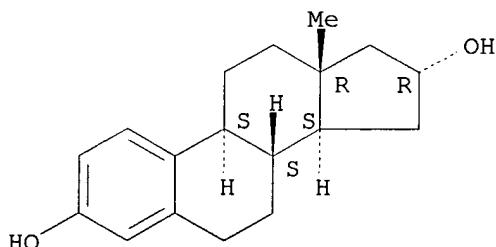
CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 1990:545540 HCPLUS
 DOCUMENT NUMBER: 113:145540
 TITLE: Activation of 'immediate-early' genes by estrogen is not sufficient to achieve stimulation of DNA synthesis in rat uterus
 AUTHOR(S): Persico, Eliana; Scalona, Marilina; Cicatiello, Luigi; Sica, Vincenzo; Bresciani, Francesco; Weisz, Alessandro
 CORPORATE SOURCE: Prima Fac. Med. Chir., Univ. Napoli, Naples, I-80138, Italy
 SOURCE: Biochemical and Biophysical Research Communications (1990), 171(1), 287-92
 CODEN: BBRCA9; ISSN: 0006-291X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 17.beta.-Estradiol, a long acting estrogen that is mitogenic for rat uterus in vivo, or the short acting estrogens estriol and 16.alpha.-estradiol, not mitogenic on their own, were injected into adult, castrated rats and their effects on uterine gene expression and rate of DNA synthesis were compared. All compds. increased steady-state mRNA concn. of c-fos, c-jun and c-myc proto-oncogenes to comparable levels (2 h after treatment), whereas only 17.beta.-estradiol stimulated DNA synthesis (20-22 h later). Based on the different retention time of the tested estrogens in rat tissues, it is concluded that a short exposure to the hormone is sufficient to render uterine cells competent to progress through the cell cycle, via activation of immediate-early genes expression, but that stimulation of DNA synthesis requires further changes, achieved via a prolonged exposure of the cells to the estrogenic stimulus.
 IT 1090-04-6, 16.alpha.-Estradiol
 RL: BIOL (Biological study)
 (immediate early gene activation by, in uterus, DNA formation independent of)
 RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

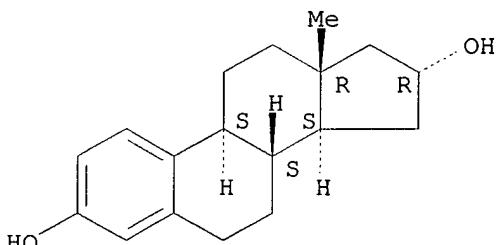


L5 ANSWER 33 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1990:152134 HCPLUS
 DOCUMENT NUMBER: 112:152134
 TITLE: Regulation of prolactin gene transcription in vivo: interactions between estrogen, pimozide, and .alpha.-ergocryptine
 AUTHOR(S): Shull, James D.; Gorski, Jack

CORPORATE SOURCE: Eppley Inst. Cancer Res., Univ. Nebraska, Omaha, NE, 68105, USA
 SOURCE: Molecular Pharmacology (1990), 37(2), 215-21
 CODEN: MOPMA3; ISSN: 0026-895X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A single injection of pimozide, a dopamine antagonist, rapidly stimulated prolactin (PRL) gene transcription in male rats, whereas an injection of .alpha.-ergocryptine, a dopamine agonist, rapidly inhibited PRL gene transcription. Pretreatment with cycloheximide blocked the induction of PRL gene transcription by pimozide but had no effect on the inhibition of transcription by ergocryptine. The interactions between ergocryptine and 16.alpha.-estradiol, an estrogen that stimulates PRL gene transcription through two independent mechanisms, were also exampd. Pretreatment with ergocryptine had no effect on the ability of 16.alpha.-estradiol to stimulate PRL gene transcription through a mechanism that is most probably mediated directly by the anterior pituitary estrogen receptor. However, ergocryptine pretreatment did block the ability of 16.alpha.-estradiol to stimulate transcription through a second, indirect, mechanism. This ergot alkaloid also blocked the ability of pimozide to stimulate PRL gene transcription. Pretreatment with 16.alpha.-estradiol had no effect on the ability of ergocryptine to inhibit PRL gene transcription, indicating that this estrogen did not grossly alter the responsiveness of the anterior pituitary to the dopamine agonist. The similarities between the effects of 16.alpha.-estradiol, via the indirect mechanism, and pimozide on PRL gene transcription suggest that estrogen may stimulate PRL gene transcription in vivo in part by reducing the release of dopamine from hypothalamic neurons.

IT 1090-04-6, 16.alpha.-Estradiol
 RL: BIOL (Biological study)
 (prolactin gene transcription stimulation by, dopamine mediation of)
 RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 34 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1990:801 HCPLUS
 DOCUMENT NUMBER: 112:801
 TITLE: Relative mitogenic activities of various estrogens and antiestrogens
 AUTHOR(S): Stack, Gary; Korach, Kenneth; Gorski, Jack
 CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA
 SOURCE: Steroids (1989), 54(2), 227-43

CODEN: STEDAM; ISSN: 0039-128X

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The abilities of a variety of estrogens and antiestrogens to stimulate DNA synthesis in the prepuberal rat uterus were compared. One microgram of each compd. was administered in vivo via a single i.p. injection. DNA synthesis was assayed in vitro in isolated nuclei 24 h later. The relative mitogenicities of the steroidal estrogens were :
 16.alpha.-estradiol < 17.alpha.-estradiol = estriol (I) = 16-epiestriol <
 16.beta.-estradiol = 17.beta.-estradiol (II). The potencies of several nonsteroidal estrogens were also tested. Indenestrol A was as potent as II, whereas indanestrol and dimethylstilbestrol had weaker activities. The antiestrogens, nafoxidine and 4-hydroxytamoxifen, were both potent stimulators of DNA synthesis. The abilities of an estrogen to stimulate increases in uterine wet wt., DNA polymerase .alpha. activities, and DNA synthesis in uterine nuclei 24 h after injection were closely correlated. Because the magnitude of the stimulation of DNA synthesis was greatest, its measurement is the most sensitive of these assays, of uterotrophic activity.

IT 1090-04-6, 16.alpha.-Estradiol 1225-58-7,

16.beta.-Estradiol

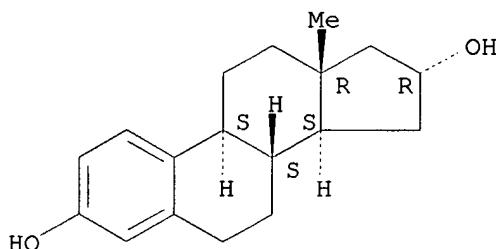
RL: PROC (Process)

(mitogenic action of, on uterus, mol. structure in relation to)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

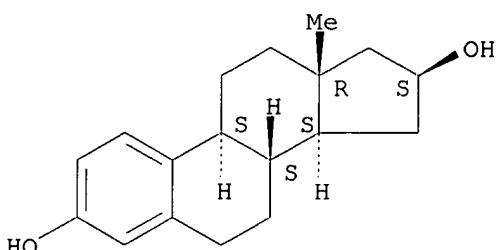
Absolute stereochemistry.



RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

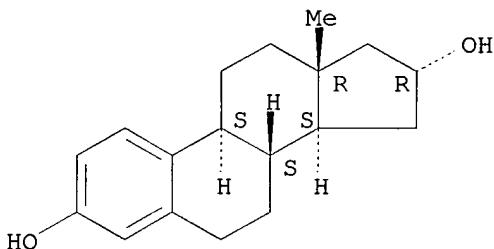
Absolute stereochemistry.



L5 ANSWER 35 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1989:471237 HCPLUS
 DOCUMENT NUMBER: 111:71237
 TITLE: Binding of radiolabeled estrogens by human cells in vitro: implications to the development of a new diagnostic and therapeutic modality in the treatment of malignancies with estrogen receptors
 AUTHOR(S): Anderson, Robert E.; Holt, John A.
 CORPORATE SOURCE: Chicago Lying-In Hosp., Univ. Chicago, Chicago, IL, 60637, USA
 SOURCE: Gynecologic Oncology (1989), 34(1), 80-3
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB An in vitro technique was employed to demonstrate the binding of Auger electron-emitting nuclide-labeled estrogenic compds. by a variety of human cell types. Human granulosa cells, endometrium, and MCF-7 breast cancer cells were incubated with either 16.alpha.-[125I]iodoestradiol or 16.alpha.-[123I]iodoestradiol in vitro. Autoradiog. techniques were subsequently utilized and revealed that binding of these estrogenic compds. by all 3 types of cells did occur and that this binding was inhibited by excess unlabeled estradiol. Histol. examn. was not able to demonstrate nuclear-specific binding in all instances, however. These compds. are potentially useful in both diagnostic and therapeutic settings and this study is the first to provide such data from human tissue.
 IT 1090-04-6D, derivs., labeled with iodine-125 and iodine-123
 RL: PROC (Process)
 (receptor binding of, in mammary carcinoma and ovary endometrium and granulosa cell of human)
 RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 36 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1988:622771 HCPLUS
 DOCUMENT NUMBER: 109:222771
 TITLE: Effect of endogenous and synthetic sex steroids on the clearance of antibody-coated cells
 AUTHOR(S): Schreiber, A. D.; Nettl, F. M.; Sanders, M. C.; King, M.; Szabolcs, P.; Friedman, D.; Gomez, F.
 CORPORATE SOURCE: Cancer Cent., Univ. Pennsylvania, Philadelphia, PA, 19104, USA
 SOURCE: Journal of Immunology (1988), 141(9), 2959-66
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB An exptl. model developed in the guinea pig, was used to study the effects of female sex hormones on macrophage clearance of IgG- and IgM-coated erythrocytes in the spleen and liver. Progesterone, its naturally occurring analog 17-hydroxyprogesterone, and its synthetic analog 16-methylprogesterone inhibited the clearance of IgG-coated erythrocytes by splenic macrophages. Furthermore, when splenic macrophages were isolated from progesterone-treated animals they expressed decreased Fc. γ R activity. Estradiol, estriol, and the estrogen analog 1,3,5(10)-estratriene-3,16 β -diol enhanced splenic macrophage clearance of IgG-coated erythrocytes. This action of the estrogens could be partially inhibited by the antiestrogen tamoxifen. However, estradiol did not affect the C3-dependent clearance of IgM-coated erythrocytes by hepatic macrophages. Concurrent administration of estradiol and progesterone demonstrated that the action of estradiol was predominant. Thus, female sex hormones alter splenic macrophage Fc. γ R function at concns. obsd. during the human menstrual cycle and pregnancy. This result may also explain alteration of disease activity in some human immunol. disorders during changes in the hormonal states.

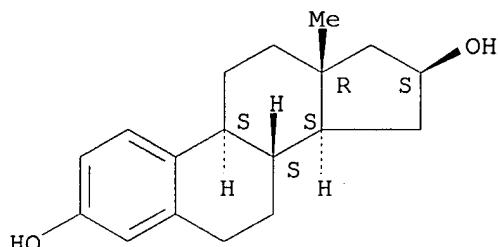
IT 1225-58-7

RL: BIOL (Biological study)
(IgG-coated erythrocyte clearance by spleen macrophage stimulation by)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16 β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 37 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1988:124686 HCAPLUS

DOCUMENT NUMBER: 108:124686

TITLE: Nuclear estrogen receptor molecular heterogeneity in the mouse uterus

AUTHOR(S): Golding, Thomas S.; Korach, Kenneth S.

CORPORATE SOURCE: Natl. Inst. Health, Natl. Inst. Environ. Health Sci., Research Triangle Park, NC, 27709, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1988), 85(1), 69-73

CODEN: PNASA6; ISSN: 0027-8424

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Holomeric estrogen receptor (ER) prep'd. from ovariectomized mouse uteri displays heterogeneous electrophoretic mobility when analyzed by SDS-PAGE. ER derived from nuclei (ERn) appears as a closely spaced doublet having apparent mol. masses of 66.4 and 65 kilodaltons (kDa), whereas ER from the cytosolic compartment (ERC) has a single band of 65 kDa. Both partially

purified ERc and the 8-S form of unactivated ERc show only the 65-kDa band. The appearance of the ERn doublet is hormonally inducible, and the relative proportions of the 2 doublet bands are influenced by the type of hormone treatment, with weakly estrogenic compds. yielding the lower band as predominant whereas potent estrogens increase the proportion of the upper band. Steroid binding of the ERn doublet was detd. by [3H]tamoxifen aziridine affinity labeling of both the 66.4- and 65-kDa peptides; binding to the 65-kDa peptide was predominant. The ERn doublet displays a time dependency after estrogen administration with maximal amts. occurring in a bimodal fashion at 1 and 8 h.

IT 1090-04-6, 16.alpha.-Estradiol

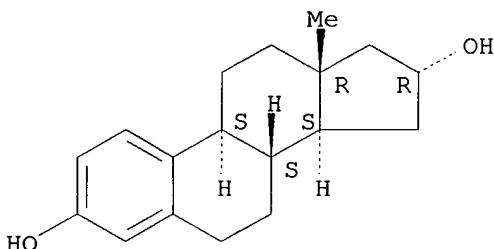
RL: BIOL (Biological study)

(estrogen receptor heterogeneity in uterus nucleus response to)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 38 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:617953 HCAPLUS

DOCUMENT NUMBER: 107:217953

TITLE: Fevicordin A and fevicordin A glucoside, novel norcucurbitacins from Fevillea cordifolia

AUTHOR(S): Achenbach, Hans; Hefter-Buebl, Ursula; Constenla, Manuel A.

CORPORATE SOURCE: Inst. Pharm., Univ. Erlangen-Nuernberg, Erlangen, D-8520, Fed. Rep. Ger.

SOURCE: Journal of the Chemical Society, Chemical Communications (1987), (6), 441-2
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fevicordin A glucoside and fevicordin A, isolated from the seeds of Fevillea cordifolia, have structures I ($\text{R} = \beta\text{-glucosyl}$) and I ($\text{R} = \text{H}$), resp., on the basis of chem. and spectral data.

IT 111250-01-2P, Fevicordin A glucoside 111250-02-3P,

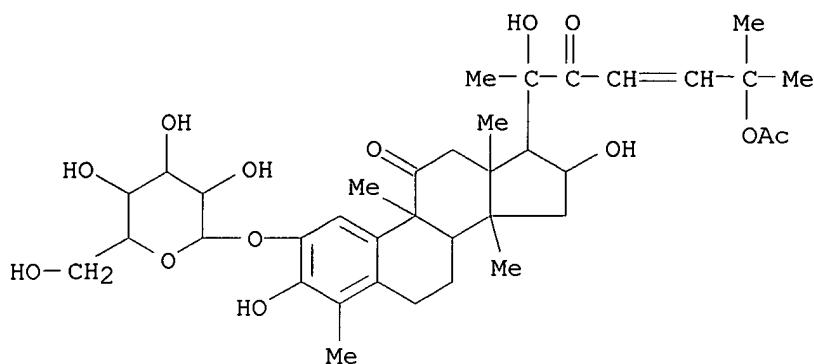
Fevicordin A

RL: PREP (Preparation)

(from Fevillea cordifolia, isolation and mol. structure detn. of)

RN 111250-01-2 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2-($\beta\text{-D-glucopyranosyloxy}$)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9. $\beta\text{,16.}\alpha\text{,23E}$)- (9CI) (CA INDEX NAME)

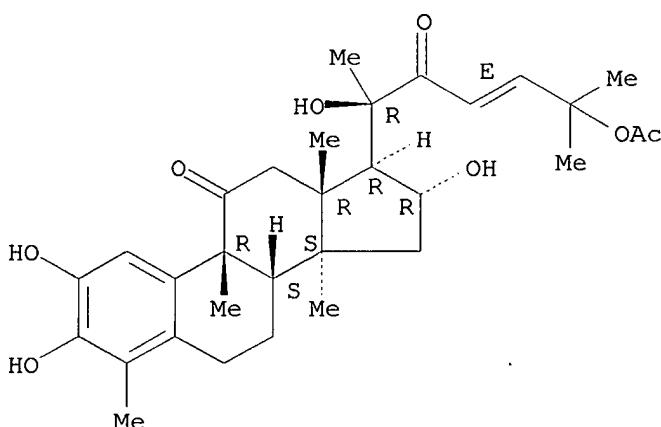


RN 111250-02-3 HCPLUS

CN 19-Norcholesta-1,3(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L5 ANSWER 39 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:96443 HCPLUS

DOCUMENT NUMBER: 106:96443

TITLE: Influence of adrenergic receptors on ovarian progesterone secretion in the pseudopregnant cat and estradiol secretion in the estrous cat

AUTHOR(S): Wheeler, A. G.; Walker, M.; Lean, J.

CORPORATE SOURCE: Dep. Physiol. Pharmacol., Univ. Queensland, St. Lucia, 4067, Australia

SOURCE: Journal of Reproduction and Fertility (1987), 79(1), 195-205

CODEN: JRPFA4; ISSN: 0022-4251

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The infusion of isoprenaline [7683-59-2] or propranolol into the abdominal aorta of the pseudopregnant cat caused an increase or decrease,

resp., in the ovarian progesterone [57-83-0] secretion rate. Apparently, the sympathetic innervation of the ovary has a physiol. influence on normal progesterone secretion, and this mechanism may explain stress-related increases in progesterone concns. The infusion of isoprenaline or propranolol after the stimulation of follicular growth had no consistent or convincing effect on estradiol [1225-58-7] secretion.

IT 1225-58-7

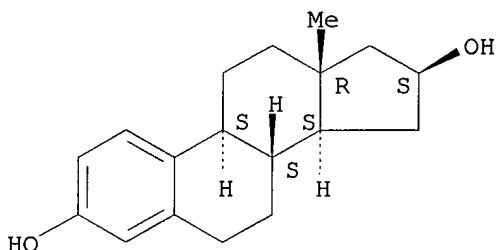
RL: PROC (Process)

(secretion of, by ovary, adrenergic receptors in relation to)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 40 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:16187 HCAPLUS

DOCUMENT NUMBER: 106:16187

TITLE: Methylcholanthrene: a possible pseudosubstrate for adrenocortical 17.alpha.-hydroxylase and aryl hydrocarbon hydroxylase

AUTHOR(S): Hornsby, Peter J.; Aldern, Kathy A.; Harris, Sandra E.

CORPORATE SOURCE: Sch. Med., Univ. California, La Jolla, CA, 92093, USA

SOURCE: Biochemical Pharmacology (1986), 35(19), 3209-19

CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In cultured bovine adrenocortical cells, the loss of steroid 17.alpha.-hydroxylase (I) activity was obsd. after incubation with 3-methylcholanthrene (3-MC). The suppression of I by 3-MC was rapid (50% loss of activity in 10 h at 1 .mu.m 3-MC), did not exhibit a lag period, and was not affected by cycloheximide. Direct effects of 3-MC on I were obsd. only at high concns., but the concn. for 50% loss of activity was 0.3 .mu.M when 3-MC was added for 24 h prior to assay of I. High concns. (to 40 .mu.M) of substrate (progesterone), did not affect the loss of activity due to 3-MC. Loss of I activity was specific; steroid 11.beta.-hydroxylase was unaffected and cell growth was unaltered. However, 22-amino-23,24-bisnorchol-5-en-3.beta.-ol, an inhibitor of I, partially prevented the loss of I at 1-30 nM. 3-MC was thought to induce cytochrome P 450s via a receptor with high affinity for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). TCDD was without effect on I over the range 10 nM-10 .mu.M. Benz[a]anthracene, 7,12-dimethylbenz[a]anthracene, benzo[a]pyrene, chrysene, and methylphenanthrenes suppressed I at high concns. (10-50 .mu.M for 50% loss of activity). Some steroids that lack a substituent at position 17 also

caused loss of I. Like I, bovine adrenocortical cell aryl hydrocarbon hydroxylase (II) was found to be suppressed by exposure to 3-MC. Compds. that caused loss of I caused loss of II, with a similar order of potency and at similar concns. Suppression of II by 3-MC did not require protein synthesis and was prevented by an inhibitor of enzymic activity, .alpha.-naphthoflavone. This implied a degree of similarity of the cytochrome P 450s for I and II, but the activities were shown to be likely due to different enzymes. The suppression of I and II by 3-MC appeared not to occur by a receptor-mediated mechanism but to be similar to the suppression of steroid 11.beta.-hydroxylase and steroid 21-hydroxylase by steroid pseudosubstrates previously obsd.

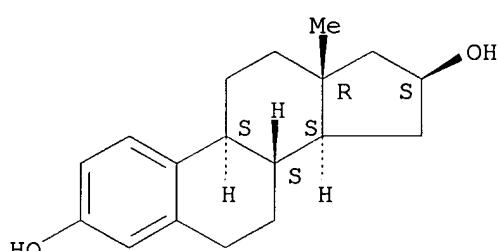
IT 1225-58-7, Estra-1,3,5(10)-triene-3,16.beta.-diol

RL: BIOL (Biological study)
(aryl hydrocarbon hydroxylase and steroid 17.alpha.-hydroxylase response to, in adrenocortical cells)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 41 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1986:475395 HCAPLUS

DOCUMENT NUMBER: 105:75395

TITLE: Comparison of immunochemical and radioligand binding assays for estrogen receptors in human breast tumors

AUTHOR(S): Di Fronzo, Giovanni; Miodini, Patrizia; Brivio, Moreno; Cappelletti, Vera; Coradini, Danila; Granata, Giovanna; Ronchi, Enrico

CORPORATE SOURCE: Ist. Nazi. Stud. Cura Tumori, Milan, 20133, Italy

SOURCE: Cancer Research (1986), 46(8, Suppl.), 4278S-4281S

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new enzyme immunoassay (EIA) for estrogen receptors (ER) was compared with conventional radioligand binding assays (multipoint dextran-coated charcoal assay for cytoplasmic ER and hydroxylapatite exchange assay for nuclear ER). Cytoplasmic ERs were measured in human breast cancer specimens by EIA and by 5-point Scatchard anal. The correlation between the 2 assays yielded a straight line with a slope of 0.92; conversely, in nuclear salt exts., linear regression anal. of hydroxylapatite exchange assay data with EIA showed a clear correlation but a slope of 1.7, demonstrating that EIA detects more ER sites. The binding of the antibody to the cytoplasmic ER mols. was investigated by sucrose d. gradient anal., which showed that EIA recognizes both cytoplasmic forms (9 and 3 S), but does not distinguish between them. Advantages and drawbacks of this

method are discussed with respect to its application for routine receptor detn. for clin. management of breast cancer patients.

IT 1090-04-6D, receptor complexes

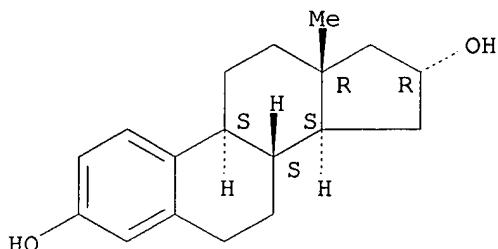
RL: ANT (Analyte); ANST (Analytical study)

(detn. of, in mammary carcinoma of human by enzyme immunoassay)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 42 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:590196 HCAPLUS

DOCUMENT NUMBER: 103:190196

TITLE: Relationship of estrogen receptors and protein synthesis to the mitogenic effect of estrogens

AUTHOR(S): Stack, Gary; Gorski, Jack

CORPORATE SOURCE: Dep. Biochem., Univ. Wisconsin, Madison, WI, 53706, USA

SOURCE: Endocrinology (1985), 117(5), 2024-32

CODEN: ENDOAO; ISSN: 0013-7227

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1,3,5(10)-Estratriene-3,16.alpha.-diol (16.alpha.-E2) [1090-04-6]

] is an estrogen which is ineffective in stimulating DNA synthesis in the prepuberal rat uterus when administered to rats in a single injection in doses up to at least 5 .mu.g. However, it acquires the same high mitogenic potency as 1,3,5(10)-estratriene-3,17.beta.-diol (17.beta.-E2) [50-28-2] if a 5-.mu.g dose is administered over 12 h via sequential injections of 1 .mu.g each at 3-h intervals. In an attempt to explain this phenomenon it was found that the ability of an estrogen to maintain a stimulated rate of protein synthesis for 12 h correlates directly with its ability to stimulate DNA synthesis. A single injection of 16.alpha.-E2 stimulates protein synthesis at 4 h to a degree comparable to 17.beta.-E2. By 12 h when the effect of 17.beta.-E2 is maximal, the effect of 1 injection of 16.alpha.-E2 had diminished to control levels. However, if 16.alpha.-E2 is administered via sequential injections at 3-h intervals, protein synthesis at 12 h is stimulated to the same extent achieved by a single injection of 17.beta.-E2. The fate of estrogen receptors in relation to these changes in protein and DNA synthesis was also examd. The effects of a single injection of 16.alpha.-E2 differ in 4 respects from those of 17.beta.-E2: the retention of receptors in the nuclear form is shorter; replenishment of receptors to the cytosolic form is more rapid and > 80% complete within 3 h; fewer receptors are processed, i.e. the loss of receptors detectable by exchange assay is smaller; and the overshoot in receptor replenishment 24 h after an injection is smaller.

Overall, the stimulation of DNA synthesis is pos. related to the rate of protein synthesis 12 h after an injection of estrogen, the retention of receptors in the nuclear form, and the amt. of receptor processing.

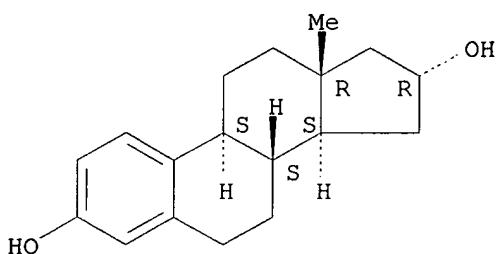
IT **1090-04-6**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(DNA formation and stimulation by, in uterus, estrogen receptor processing and protein formation in relation to)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 43 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:590195 HCAPLUS

DOCUMENT NUMBER: 103:190195

TITLE: Estrogen-stimulated deoxyribonucleic acid synthesis:
a ratchet model for the prereplicative period

AUTHOR(S): Stack, Gary; Gorski, Jack

CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI,
53706, USA

SOURCE: Endocrinology (1985), 117(5), 2017-23

CODEN: ENDOAO; ISSN: 0013-7227

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Multiple injections of a short acting estrogen, 1,3,5(10)-estratriene-3,16.alpha.-diol (16.alpha.-E2) [1090-04-6] were used to analyze the lag or prereplicative period of approx. 12 h, which precedes the onset of estradiol [50-28-2]-stimulated DNA synthesis in prepuberal rat uterus. A single injection of 1.0 .mu.g 16.alpha.-E2, which itself does not stimulate DNA synthesis, shortened by 3-4 h the lag period between subsequently administered estrogen and the initiation of DNA synthesis. This lag-shortening effect of 16.alpha.-E2 was stable for 24 h, but decayed by 36 h. One or 2 addnl. injections of 16.alpha.-E2 given sequentially at 3-h intervals each further shortened the lag period but to a lesser extent than the 1st injection. Apparently, estrogen induces the accumulation of relatively stable cell changes which are required for the onset of DNA synthesis. The prolonged estrogen requirement during the lag period is not truly discontinuous as previously suggested but rather can be satisfied by discontinuous pulses of estrogen in a ratchet-like fashion because of the stability of their effects.

IT **1090-04-6**

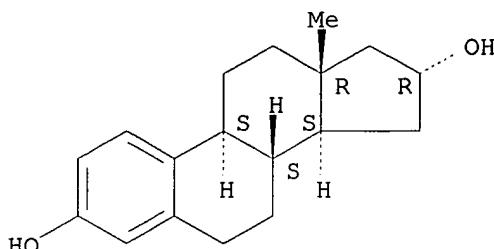
RL: BIOL (Biological study)

(DNA formation stimulation by discontinuous administration of, in uterus)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 44 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:574487 HCPLUS

DOCUMENT NUMBER: 103:174487

TITLE: Isolation of novel microbial 3.alpha.-, 3.beta.-, and 17.beta.-hydroxysteroid dehydrogenases. Purification, characterization, and analytical applications of a 17.beta.-hydroxysteroid dehydrogenase from an *Alcaligenes* sp

AUTHOR(S): Payne, Donna W.; Talalay, Paul

CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA

SOURCE: Journal of Biological Chemistry (1985), 260(25), 13648-55

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By selecting for growth on testosterone or 17.beta.-estradiol as the only source of org. C, a no. of soil microorganisms which contain highly active and novel, inducible, NAD-linked 3.alpha.-, 3.beta.-, and 17.beta.-hydroxy steroid dehydrogenases were isolated. Such enzymes are suitable for the microanal. of steroids and of steroid-transforming enzymes, as well as for performing stereoselective oxidns. and redn. of steroids. Of particular interest among these organisms is a new species of *Alcaligenes* contg. 17.beta.-hydroxy steroid dehydrogenase (I) easily separable from 3.beta.-hydroxy steroid dehydrogenase activity. Unlike any of the other isolated organisms, this *Alcaligenes* species contained no 3.alpha.-hydroxy steroid dehydrogenase activity. A large-scale purifn. (763-fold) to homogeneity of the major induced I was achieved by ion-exchange, hydrophobic, and affinity chromatogs. The enzyme has high specific activity for the oxidn. of testosterone ($V_{max} = 303 \text{ .mu.mol/min/mg protein}$; $K_m = 3.6 \text{ .mu.M}$) and reacts almost equally well with 17.beta.-estradiol ($V_{max} = 356 \text{ .mu.mol/min/mg}$; $K_m = 6.4 \text{ .mu.M}$). It consists of apparently identical subunits mol. wt. = 32,000 and exists in polymeric form under nondenaturing conditions (mol. wt. = 68,000 by gel filtration. and 86,000 by polyacrylamide gel electrophoresis). The isoelec. point is pH 5.1. The enzyme is almost completely specific for 17.beta.-hydroxy steroids which may be .DELTA.5-olefins or ring A phenols or have cis or trans A/B ring fusions. Substituents at other positions are tolerated, although the presence of a 16.alpha.- or 16.beta.-OH group blocks the oxidn. of the 17.beta.-OH function. 3.beta.-Hydroxy steroids

(A/B ring fusion trans, but not cis, or .DELTA.5-olefins) are very poor substrates. The application of this highly active, specific, and stable I to the microestn. of steroids by enzymic cycling of nicotinamide nucleotides and for the stereospecific oxidn. of steroids is demonstrated.

IT 1225-58-7

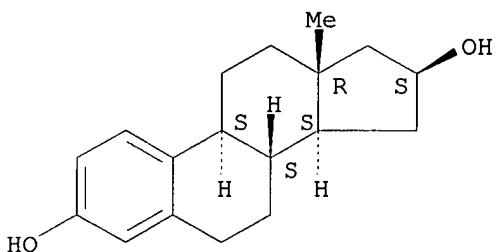
RL: BIOL (Biological study)

(17.beta.-hydroxy steroid dehydrogenase of Alcaligenes specificity for, structure in relation to)

RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 45 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:417054 HCPLUS

DOCUMENT NUMBER: 103:17054

TITLE: Estrogen regulates the transcription of the rat prolactin gene in vivo through at least two independent mechanisms

AUTHOR(S): Shull, James D.; Gorski, Jack

CORPORATE SOURCE: Dep. Biochem., Univ. Wisconsin, Madison, WI, 53706, USA

SOURCE: Endocrinology (1985), 116(6), 2456-62

CODEN: ENDOAO; ISSN: 0013-7227

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 16.alpha.-Estradiol [1090-04-6] and estriol [50-27-1] induced transcription of the rat prolactin (PRL) [9002-62-4] gene in vivo in a biphasic manner. The level of PRL gene transcription was exampd. by measuring the amt. of radiolabeled UTP incorporated into PRL-specific RNA sequences by nuclei isolated from the anterior pituitary gland at various times after hormone treatment. A single injection of 16.alpha.-estradiol stimulated PRL gene transcription within 30 min, and this initial phase of stimulated transcription was obsd. through 2 h after treatment. A 2nd phase of stimulated PRL gene transcription was obsd. by 6 h after 16.alpha.-estradiol treatment and continued through 24 h. A biphasic stimulation of PRL gene transcription also was obsd. in response to a single injection of estriol. However, the initial phase extended into the 2nd phase, and the phases were, therefore, distinguishable only by their differing levels of stimulation. The induction of the initial phase of increased PRL gene transcription by 16.alpha.-estradiol was obsd. in animals in which cycloheximide or puromycin had greatly inhibited pituitary protein synthesis. In contrast, induction of the 2nd phase of stimulated transcription by 16.alpha.-estradiol was blocked by prior cycloheximide treatment. An injection of 16.alpha.-estradiol resulted in

activation of the cytosol form of the pituitary estrogen receptor to its nuclear form, with maximal levels of nuclear form receptors being obsd. within 1 h of injection. Within 4 h of treatment, the cytosol and nuclear forms of the pituitary estrogen receptor had returned to control levels. Apparently, estrogen regulates transcription of the rat PRL gene in vivo through at least 2 independent mechanisms.

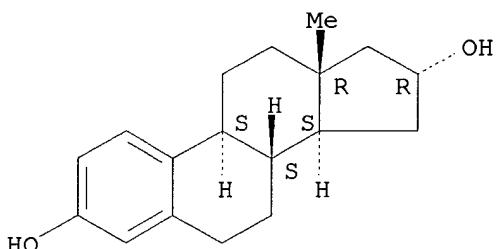
IT 1090-04-6

RL: BIOL (Biological study)
(prolactin gene transcription response to)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 46 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1984:523208 HCPLUS

DOCUMENT NUMBER: 101:123208

TITLE: Structure-binding affinity correlations for iodo- and selenoestrogen analogs and mapping of the estrogen receptor by the MTD method

AUTHOR(S): Simon, Z.; Mihalas, G. I.; Caspi, E.

CORPORATE SOURCE: Dep. Biophys., Inst. Med., Timisoara, 1900, Rom.

SOURCE: Revue Roumaine de Chimie (1984), 29(1), 83-97

CODEN: RRCHAX; ISSN: 0035-3930

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A structure-binding affinity correlation of iodo estrogen and seleno estrogen analogs was carried out by the min. topol. difference (MTD) method. A correlation coeff. $r = 0.80$ was obtained for the whole series of 30 analogs. Structure-affinity correlations were also performed for another series of estrogen and stilbestrol derivs. The attributes of the vertices of the hypermol. to the receptor cavity, wall, and exterior regions were verified by comparing the 17 common attributes for the iodo and seleno estrogens with those of the structure-affinity correlation for the sep. series of estrogen and stilbestrol derivs.: there are 13 identical and 4 different attributes, 2 of which may be explained by differences in the polar or apolar nature of atoms occupying the vertices. The estrogen receptor site should be mostly hydrophobic, with 2 groups bonding estrogenic O-atoms at, or nearby positions 3 and 17 and with some large later openings.

IT 71683-63-1 71683-69-7 71683-70-0

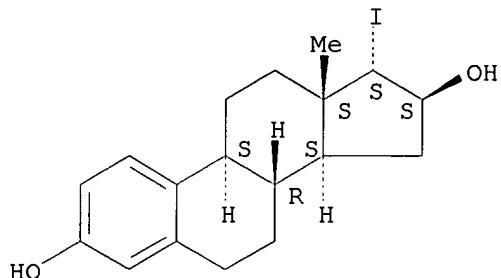
RL: BIOL (Biological study)
(estrogen receptor affinity for, structure in relation to)

RN 71683-63-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-iodo-, (16.beta.,17.alpha.)- (9CI)

(CA INDEX NAME)

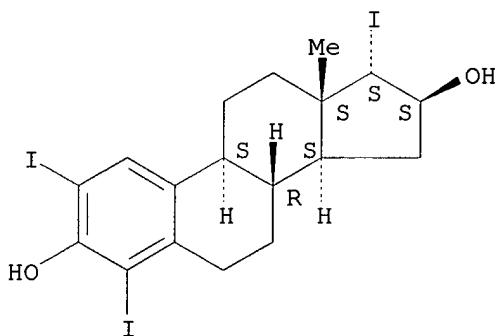
Absolute stereochemistry.



RN 71683-69-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 2,4,17-triiodo-, (16.beta.,17.alpha.)-
(9CI) (CA INDEX NAME)

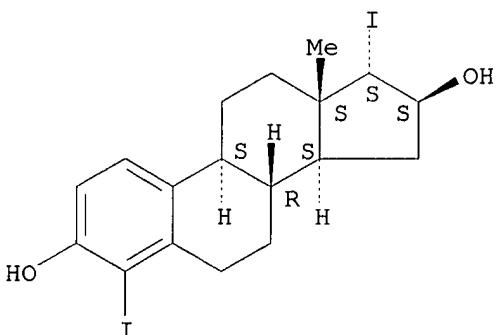
Absolute stereochemistry.



RN 71683-70-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 4,17-diiodo-, (16.beta.,17.alpha.)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 47 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1984:203914 HCPLUS
 DOCUMENT NUMBER: 100:203914
 TITLE: Primary cultures of estrogen-responsive cells from rat uteri: induction of progesterone receptors and a secreted protein
 AUTHOR(S): Kassis, Judy A.; Sakai, Dennis; Walent, Jane H.; Gorski, Jack
 CORPORATE SOURCE: Dep. Biochem., Univ. Wisconsin, Madison, WI, 53706, USA
 SOURCE: Endocrinology (1984), 114(5), 1558-66
 CODEN: ENDOAO; ISSN: 0013-7227
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Uterine cells from immature rats can be grown in culture, are estrogen responsive, and contain estrogen receptors. Progesterone [57-83-0] receptor is induced within 1 day of 17. β -estradiol [50-28-2] treatment, with maximal response occurring after 2 days of treatment (300-500% of the control value). Induction of progesterone receptor occurred at physiol. 17. β -estradiol concns., with half-maximal response at about 5 times. 10-11M. 17. β -Estradiol induced the synthesis of a secreted protein (mol. wt., 130,000) in a dose-dependent fashion. This 130-K protein was also induced by 16. α -estradiol [1090-04-6] (1-10 nM), but not by progesterone (10 nM), testosterone (1 nM), or dexamethasone (1 nM). Examn. of the estrogen-binding properties of the cultured cells shows a saturable binding site (K_d , .apprx.10-10M) which can be translocated to the nucleus. Estrogen receptors were maintained at in vivo levels as uterine cells proliferated throughout 10 days of culture. This was in contrast to estrogen receptor levels in Fischer 344 rat pituitary cell cultures, which dropped off drastically on a DNA basis as cells proliferated. Thus, estrogen receptor-contg. rat uterine cells proliferate and are responsive in primary cell cultures.

IT 1090-04-6

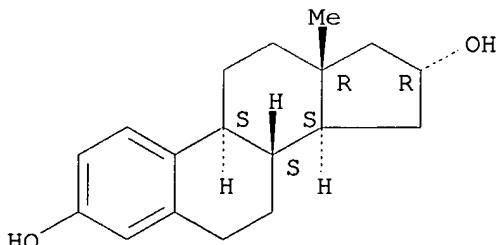
RL: BIOL (Biological study)

(protein formation response to, in uterus cell in culture)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. α .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 48 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1984:47664 HCPLUS

DOCUMENT NUMBER: 100:47664

TITLE: Inhibitor specificity of the placental microsomal

oxidase system responsible for the aromatization of epitestosterone (17.alpha.-hydroxy-4-androsten-3-one)

Sheean, Leon A.; Meigs, Robert A.

AUTHOR(S):
CORPORATE SOURCE:
Sch. Med., Case Western Reserve Univ., Cleveland, OH,
44106, USA

SOURCE: Steroids (1983), 41(2), 225-41
CODEN: STEDAM; ISSN: 0039-128X

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Human placental microsomes converted epitestosterone to 17.alpha.-estradiol at rates of 23-48 pmol/min/mg protein with a Km of 113 .mu.M. The activity was inhibited 70-90% by concns. of CO, metyrapone, octylamine, 7,8-benzoflavone, and 7-ethoxycoumarin which had no effect on the aromatization of 4-androstene-3,17-dione. Conversely, CN- and N3- were more effective inhibitors of the conversion of the latter androgen. A variety of neutral steroids inhibited the aromatization of epitestosterone with 19-norsteroids being particularly effective, but competitive effects could not be demonstrated. Both 17.beta.-hydroxy-4-estren-3-one and 16.alpha.-hydroxy-4-androstene-3,17-dione caused a mixed inhibition. A no. of phenolic steroids were also inhibitory with 16-oxo compds. being particularly effective. Inhibition by estrone was non-competitive ($K_i = 16 \mu M$). The aromatization of epitestosterone resembles placental microsomal oxidase activities against estrone and benzo[a]pyrene in its inhibitor specificity and epitestosterone may be the native substrate for an oxidase also active in the metab. of arom. xenobiotic chems.

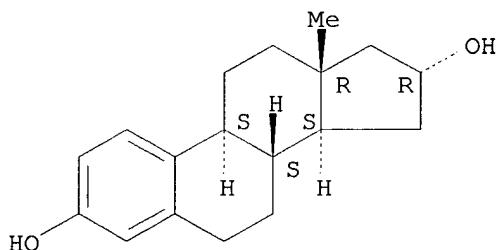
IT 1090-04-6 1225-58-7

RL: BIOL (Biological study)
(epitestosterone oxidase of human placenta microsomes inhibition by)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

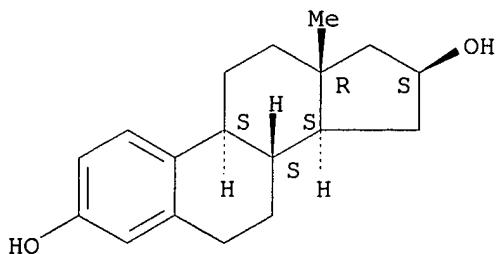
Absolute stereochemistry.



RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 49 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1982:568926 HCAPLUS
 DOCUMENT NUMBER: 97:168926
 TITLE: Compositions inhibiting estrogen sulfotransferase activity
 INVENTOR(S): Brooks, Samuel C.
 PATENT ASSIGNEE(S): Wayne State University, USA
 SOURCE: U.S., 11 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

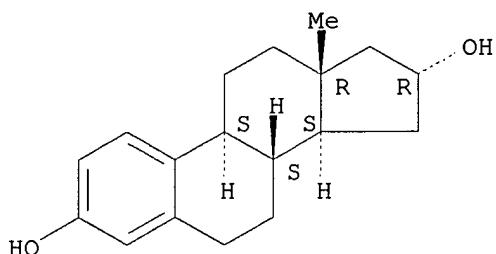
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4340602	A	19820720	US 1978-952592	19781018
US 4810700	A	19890307	US 1983-495221	19830518
PRIORITY APPLN. INFO.:			US 1978-952592	19781018
			US 1982-355806	19820308

AB estrogen sulfotransferase (I) [9032-76-2] inhibitor compns. (oral, vaginal or topical), consisting of II (R1 = Br, NO₂ or H; R2 = Br, NO₂, NH₂ or H; R = H or C1-4 alkyl; R3 = O or H₂; R4 = H₂, O, or .alpha.-H and .beta.-OH) in admixts. with pharmaceutical carriers, are useful for the termination of pregnancy by preventing implantation of a blastocyst in the epithelial uterine lining of mammalian females. Thus, an ointment was prep'd. contg. 2,4-dinitro-1,3,5-(10)-estratriene-3,17.beta.-diol (II, R1 = R2 = NO₂, R = H, R3 = H₂, R4 = .alpha.-H,.beta.-OH) [20823-11-4], liq. petrolatum 250, wool fat 200 and white petrolatum q.s. ad 1000 g. The I inhibitory activity of II was demonstrated. Estrogen metab. is discussed in relation II.

IT 1090-04-6
 RL: BIOL (Biological study)
 (estrogen sulfotransferase inhibition by)

RN 1090-04-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 50 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1982:193649 HCAPLUS

DOCUMENT NUMBER: 96:193649

TITLE: Biologic activity of the iodoestrogens and their use
in breast cancer

AUTHOR(S): Longcope, C.; Arunachalam, T.; Rafkind, I.; Caspi, E.

CORPORATE SOURCE: Worcester Found. Exp. Biol., Shrewsbury, MA, 01545,
USASOURCE: Advances in Experimental Medicine and Biology (1982),
138(Horm. Cancer), 191-210

CODEN: AEMBAP; ISSN: 0065-2598

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The iodinated estrogens 6-iodoestra-1,3,5(10),6-tetraene-3,17.beta.-diol [71696-92-9], 16.alpha.-iodoestradiol [71765-94-1], and 16.beta.-iodoestradiol [71696-91-8] displaced [³H]estradiol from rabbit uterine cytosol receptor by competitive inhibition. The 3 compds. translocated cytosol receptor to the nucleus in vitro and increased mouse uterine wt. in vivo. Relative activity was of the order 16.alpha.- > 16.beta.- > 6-iodo deriv. 16.alpha.-[¹²⁵I]iodoestradiol (I) [71765-93-0] bound with a high affinity to the 8 s cytosol receptor. Administration of I to rats resulted in high levels of radioactivity in the uterus, liver, and thyroid, but only in liver and thyroid following 6-[¹²⁵I]iodoestratetraene (II) [78271-51-9]. II administration to DMBA-induced mammary tumor-bearing rats resulted in radioactive imaging of tumors. I had no such effect. Radioactivity was assocd. with nonspecific 4 s proteins. Iodoestrogens are proposed as potential imaging agents.

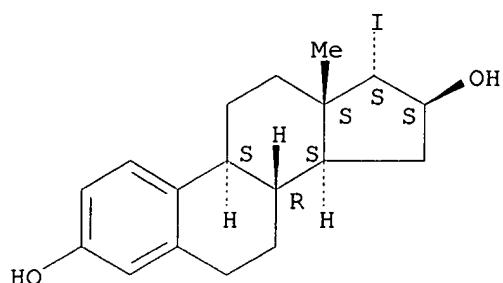
IT 71683-63-1 71683-69-7 71683-70-0

RL: BIOL (Biological study)
(uterus cytosol binding of)

RN 71683-63-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-ido-, (16.beta.,17.alpha.)- (9CI)
(CA INDEX NAME)

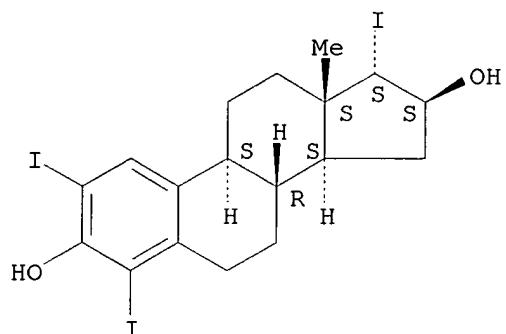
Absolute stereochemistry.



RN 71683-69-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 2,4,17-triiodo-, (16.beta.,17.alpha.)-
(9CI) (CA INDEX NAME)

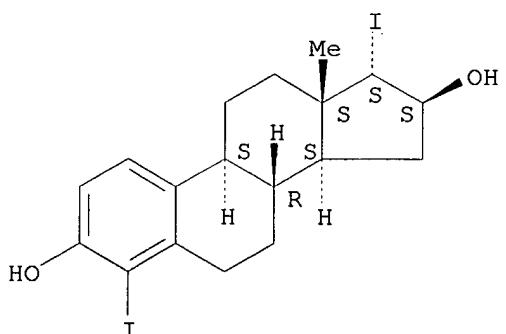
Absolute stereochemistry.



RN 71683-70-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 4,17-diiodo-, (16.beta.,17.alpha.)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 51 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1981:561659 HCPLUS

DOCUMENT NUMBER: 95:161659

TITLE: Characteristics of membrane transport of methotrexate

AUTHOR(S): by cultured human breast cancer cells
 Schilsky, Richard L.; Bailey, Brenda D.; Chabner,
 Bruce A.

CORPORATE SOURCE: Div. Cancer Treat., Natl. Cancer Inst., Bethesda, MD,
 20205, USA

SOURCE: Biochemical Pharmacology (1981), 30(12), 1537-42
 CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

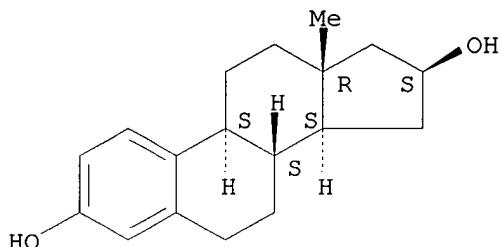
LANGUAGE: English

AB Methotrexate (I) [59-05-2] transport by MCF-7 cells and cultured estrogen- and insulin [9004-10-8]-sensitive human breast cancer cells exhibited a high-affinity carrier system that displayed Michaelis-Menten kinetics (K_m 8.22. μ M, V_{max} 12.22 nmol/min/g cell protein), was competitively inhibited by leucovorin and aminopterin but not folic acid, and was temp.-sensitive (Q_{10} 2.25). Initial uptake rates were not affected by ouabain or NaN₃, but efflux of intracellular drug was markedly inhibited by NaN₃, suggesting an energy-dependent efflux mechanism. A low affinity uptake component was identified with extracellular $I > 10.\mu$ M, possibly representing a lower affinity membrane carrier or passive diffusion. Growth of MCF-7 cells in serum-free medium induced an increase in K_m to 15.93. μ M; insulin, but not estradiol, reversed this change. Thus, I transport in this human solid tumor is similar to that in human leukemia cells.

IT 1225-58-7
 RL: BIOL (Biological study)
 (methotrexate transport by breast cancer cells response to)

RN 1225-58-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 52 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1981:528546 HCAPLUS
 DOCUMENT NUMBER: 95:128546
 TITLE: High-performance liquid chromatography of naturally occurring estrogens
 AUTHOR(S): Lin, Jiann-Tsyh; Heftmann, Erich
 CORPORATE SOURCE: West. Reg. Res. Cent., Sci. Educ. Admin., Berkeley,
 CA, 94710, USA
 SOURCE: Journal of Chromatography (1981), 212(2), 239-44
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Free naturally occurring estrogens were sep'd. by adsorption and reversed-phase high-performance liq. chromatog. (HPLC) with UV detection.

Adsorption HPLC was carried out on a 250 times. 4.6 mm stainless-steel column packed with Zorbax BP-SIL. Reversed-phase HPLC was carried out on a column of the same dimensions packed with Zorbax BP-ODS. For adsorption HPLC of the more polar estrogens, n-hexane-EtOH (9:1) was used as the eluent, and the system resolved 3 of the 4 epimeric estriols (16-epiestriol, estriol, and 16,17-epiestriol) but did not sep. 16-epiestrol from 17-epiestriol. The latter pair was resolved by reversed-phase HPLC with MeCN-H₂O (35:65) as the eluent, but the other epimers could not be sep'd. this way. On the other hand, the position isomers, estriol and 6.α-hydroxyestradiol, which could not be sep'd. by adsorption HPLC, were resolved by reversed-phase HPLC. For adsorption HPLC of the less polar estrogens, n-hexane-EtOH (97:3) was used. This eluent sep'd. well monoools and diols but did not sep. estrone from 6-dehydroestrone and 7.α-dihydroequilin from 3,16.α-estradiol. These 2 pairs were sep'd. by reversed-phase HPLC with MeCN-H₂O (35:65). In general, reversed-phase HPLC was superior to adsorption HPLC in the sepn. of estrogens differing from each other by a double bond.

IT 1090-04-6

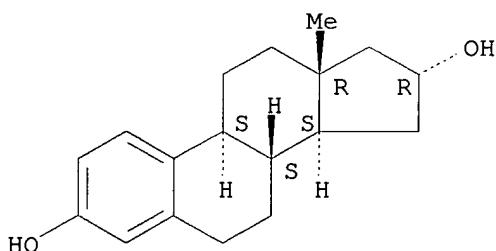
RL: ANT (Analyte); ANST (Analytical study)

(chromatog. of, adsorption and reversed-phase high-performance liq.)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.α.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 53 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1981:474107 HCPLUS

DOCUMENT NUMBER: 95:74107

TITLE: Estrogen receptor replenishment. Evidence for receptor recycling

AUTHOR(S): Kassis, Judy A.; Gorski, Jack

CORPORATE SOURCE: Dep. Biochem., Univ. Wisconsin, Madison, WI, 53706, USA

SOURCE: Journal of Biological Chemistry (1981), 256(14), 7378-82

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Replenishment of uterine estrogen receptor was examd. in immature rats following injection of 16.α.-estradiol [1090-04-6]. 16.α.-Estradiol, after a single injection, stimulated early estrogenic responses (water imbibition, induced protein synthesis, etc.), but not long-term responses (DNA synthesis). Estrogen receptor replenishment after 16.α.-estradiol injection was complete within 4 h. Furthermore, disappearance of receptor from the nucleus closely corresponded to a

reappearance of receptor in the cytoplasm. In contrast to this, receptor replenishment following injection of 1 .mu.g of either diethylstilbestrol [56-53-1] or 17.beta.-estradiol [50-28-2] was very slow and lagged behind the disappearance of nuclear receptor, leading to an apparent decrease in total receptor content. Half-lives for the clearance of nuclear estrogen-receptor complexes were 30 min for 16.alpha.-estradiol and 2 h for 17.beta.-estradiol, resp. Inhibition of protein synthesis by cycloheximide did not inhibit replenishment after 16.alpha.-estradiol injection. Multiple injections of 16.alpha.-estradiol did not lead to a lag in replenishment time or a decrease in total receptor content. Estrogen receptor replenishment appears to be due entirely to receptor recycling.

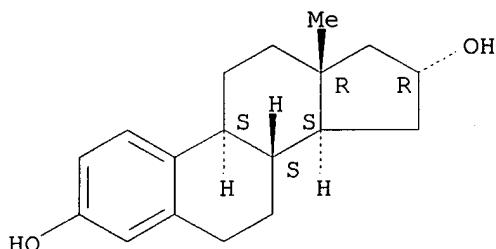
IT 1090-04-6

RL: BIOL (Biological study)
(estrogen receptor replenishment response to, in uterus)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 54 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1980:16018 HCPLUS

DOCUMENT NUMBER: 92:16018

TITLE: Iodoestrogens, syntheses, and interaction with uterine receptors

AUTHOR(S): Arunachalam, Thangavel; Longcope, Christopher; Caspi, Eliah

CORPORATE SOURCE: Worcester Found. Exp. Biol., Shrewsbury, MA, 01545, USA

SOURCE: Journal of Biological Chemistry (1979), 254(13), 5900-5

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The model syntheses of a no. of nonradioactive iodo estrogen analogs are described. The analogs were tested for their ability to displace (compete with) tritium-labeled estradiol [50-28-2] from receptor sites in the rat uterus. The most active compds., 16.beta.-iodoestra-1,3,5(10)-triene-3,17.beta.-diol (I) [71696-91-8] and 6-iodoestra-1,3,5(10),6-tetraene-3,17.beta.-diol (II) [71696-92-9], showed a relative binding affinity of 0.57 and 0.49, resp.

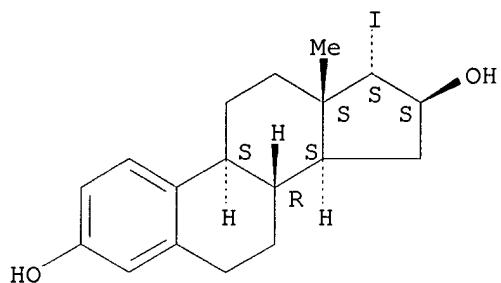
IT 71683-63-1P 71683-69-7P 71683-70-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. and estradiol receptor binding of)

RN 71683-63-1 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-iodo-, (16.beta.,17.alpha.)- (9CI)
 (CA INDEX NAME)

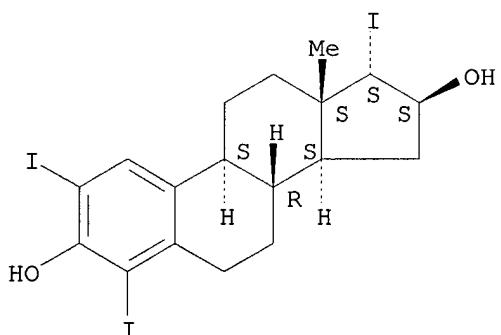
Absolute stereochemistry.



RN 71683-69-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 2,4,17-triiodo-, (16.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

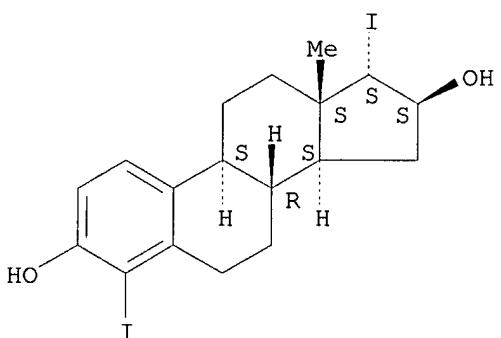
Absolute stereochemistry.



RN 71683-70-0 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 4,17-diiodo-, (16.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 55 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1979:604887 HCAPLUS
 DOCUMENT NUMBER: 91:204887
 TITLE: Synthesis and estrogenic properties of
 17-epi-ethynodiol and its ether derivatives
 epimestranol and epiquinestrol
 AUTHOR(S): Kanojia, Ramesh M.; Allen, George O.; Killinger,
 Joanne M.; McGuire, J. L.
 CORPORATE SOURCE: Div. Chem. Res., Ortho Pharm. Corp., Raritan, NJ,
 08869, USA
 SOURCE: Journal of Medicinal Chemistry (1979), 22(12), 1538-41
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The title compds. I (R = H, Me, or cyclopentyl) were prep'd. and evaluated for oral estrogenic properties by ureotrophic assay in immature rats, cornification values in ovariectomized, mature rats, and by in vitro binding affinity for the rabbit uterine estrogen receptor. 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol [4717-38-8] showed moderate binding affinity for the estrogen receptor, but failed to elicit ureotrophic response even at 10 mg/kg and was inactive as an antiestrogen at 3 mg/kg.

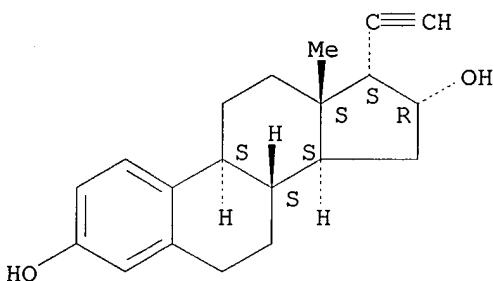
IT 71683-07-3P 71698-88-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 71683-07-3 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16-diol, (16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

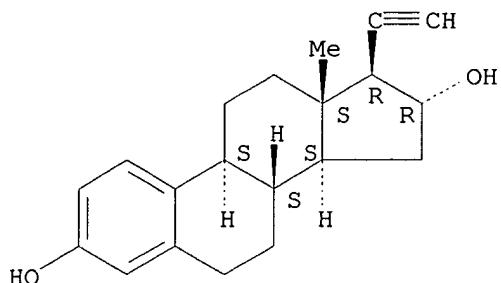
Absolute stereochemistry.



RN 71698-88-9 HCAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 56 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1979:66957 HCPLUS

DOCUMENT NUMBER: 90:66957

TITLE: Unique steroid congeners for receptor studies

AUTHOR(S): Ojasoo, Tieu; Raynaud, Jean Pierre

CORPORATE SOURCE: Cent. Rech., Roussel-UCLAF, Romainville, Fr.

SOURCE: Cancer Research (1978), 38(11, Pt. 2), 4186-98

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple in vitro system was used to define the mol. requirements for a highly specific interaction between a steroid and the receptor corresponding to a single class of hormone. Homogenates or crude 105,000 g supernatant were prep'd. from the target organs considered as end points in routine biol. potency tests. Available radioligands not bound by plasma proteins (tags) were used to single out the receptors. For each receptor singled out in the target organ cytoplasm, the ability of >700 mols. to decrease bound radioactivity was compared to that of the natural hormone (relative. binding affinity) with the use of a dextran-coated charcoal technique to sep. bound from unbound steroid. On the basis of the results of 81 mols., the effect of various substituents on the affinity and specificity of the natural hormones was detd. Mols. interacting markedly with several receptors were submitted to x-ray crystallog. in order to establish whether overlap between the various conformations of the natural hormone and of the test mol. might not partly account for lack of specificity.

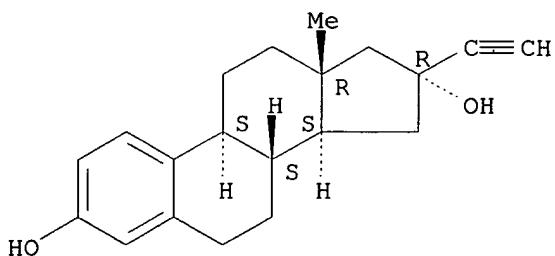
IT 24989-47-7

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(receptor binding of, structure in relation to)

RN 24989-47-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 16-ethynyl-, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 57 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1979:48715 HCPLUS

DOCUMENT NUMBER: 90:48715

TITLE: Investigation of hormone-receptor interactions by means of fluorescence labeling

AUTHOR(S): Dandiker, Walter B.; Brawn, R. James; Hsu, Mao-Lin; Brawn, Peter N.; Levin, Jacques; Meyers, Cal Y.; Kolb, Vera M.

CORPORATE SOURCE: Dep. Biochem., Scripps Clin. Res. Found., La Jolla, CA, USA

SOURCE: Cancer Research (1978), 38(11, Pt. 2), 4212-24
CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Scatchard plots from fluorescence polarization with estrone (I) [53-16-7] labeled with fluorescein at position 17 were hyperbolic and consistent with 2 classes of binding sites having assocn. consts. 5.6 .times. 1010 and 6.4 .times. 107 M-1 in the rat uterine cytosol. Binding by high-affinity sites, which were present at .apprx.3 times the concn. of specific sites (radiometric dextran-coated charcoal assay), was abrogated by estradiol [50-28-2] or diethylstilbestrol [56-53-1]. Kinetic measurements showed that binding sites that can be blocked by excess estradiol or diethylstilbestrol are those that are both slowly assocg. and slowly dissocg. Staining of tissues by I labeled with fluorescein at position 17 as seen in the fluorescence microscope showed specificity. In normal rat uterus only epithelial cells were stained. In 1 human infiltrating ductal carcinoma only the malignant ductoid elements stained, whereas in another there was essentially no staining.

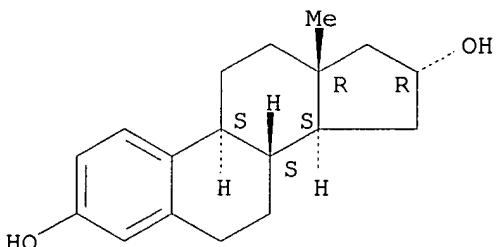
IT 1090-04-6

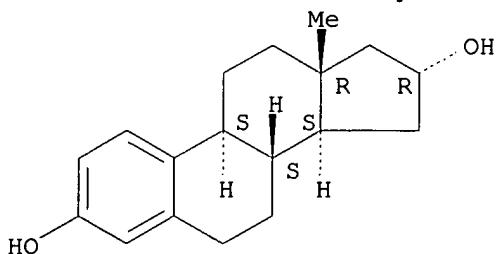
RL: PROC (Process)
(estrogen receptor binding of)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L5 ANSWER 58 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1978:116912 HCAPLUS

DOCUMENT NUMBER: 88:116912

TITLE: Inhibition of human placental 17. β -hydroxysteroid dehydrogenase by steroids and nonsteroidal alcohols: aspects of inhibitor structure and binding specificity

AUTHOR(S): Blomquist, Charles H.; Kotts, Claire E.; Hakanson, Erick Y.

CORPORATE SOURCE: Dep. Obstet. Gynecol., St. Paul-Ramsey Hosp., St. Paul, MN, USA

SOURCE: Archives of Biochemistry and Biophysics (1978), 186(1), 35-41

CODEN: ABBIA4; ISSN: 0003-9861

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Inhibition of human placental 17. β -hydroxysteroid dehydrogenase by C18 and C19 steroids and nonsteroidal alcs. was assayed at pH 9.0 with 17. β -estradiol 3-Me ether and NAD as reactants. The nonsteroidal alcs. tested were poor inhibitors. Cyclopentanol and cyclohexanol had Ki values >5mM. Nonarom. C18 and C19 steroids with O functions at both positions 3 and 17 gave no detectable inhibition or had Ki values .gtoreq.160 .mu.m. 3. β -Hydroxy-5,16-androstadiene, 5-androsten-3. β -ol, 1,3,5(10)-estratrien-3-ol, and 1,3,5(10),16-estratetraen-3-ol, steroids lacking a C(17) oxygen function, had Ki values of 1.8, 6.0, 0.04, and 0.17 .mu.M, resp., demonstrating that both C18 and C19 steroids can bind at the steroid site. Binding specificity is narrowed and binding affinity for nonarom. steroids weakened by O functions at C(17) or both C(3) and C(17). The structural implications of the specificity data for steroid recognition and complex formation and in vivo control of enzyme activity are discussed.

IT 1225-58-7

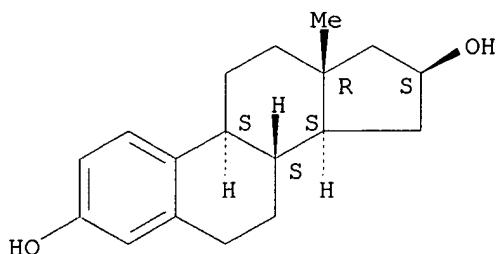
RL: BIOL (Biological study)

(17. β -hydroxysteroid dehydrogenase inhibition by, kinetics of)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 59 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:579756 HCPLUS

DOCUMENT NUMBER: 87:179756

TITLE: Studies on bovine adrenal estrogen sulfotransferase.
Inhibition and possible involvement of
adenine-estrogen stackingAUTHOR(S): Rozhin, Jurij; Huo, Anne; Zemlicka, Jiri; Brooks,
Samuel C.

CORPORATE SOURCE: Michigan Cancer Found., Detroit, MI, USA

SOURCE: Journal of Biological Chemistry (1977), 252(20),
7214-20

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The inhibition of bovine adrenal estrone sulfotransferase (I) was studied utilizing representative androgens and estrogens with structural changes in rings A, B, and D. These investigations showed O functions in positions 3, 16, or 17 to be required for the binding of estrogens or androgens to I. 5.alpha.-Androstanes (all trans-fused rings) were weak noncompetitive inhibitors and bound more tightly than the 5.beta. isomers (cis-fused A and B rings). The competitive inhibition obsd. with the estrogens did not require a free 3-phenolic hydroxyl; however, groups larger than 3-methoxy limited binding. Whereas the product, estrone sulfate, was not inhibitory, phosphate esters on positions 3- or 17.beta., or a sulfate moiety on the 17.beta.-hydroxyl group of estrogens slightly inhibited I. The stacking of adenine (in adenosine 3'-phosphate-5'-phosphosulfate) with the A ring of estrogens was postulated for the enzyme-bound transition state. This structure, which facilitates the H-bonding between the 6-amino group of adenine and the 4-nitro, 4-bromo, or 6-keto substituents on estrogens, readily explained the unusual substrate and inhibitory properties of these compds. Certain of these estrogen derivs., which possessed little or no hormonal activity, were efficient inhibitors of I.

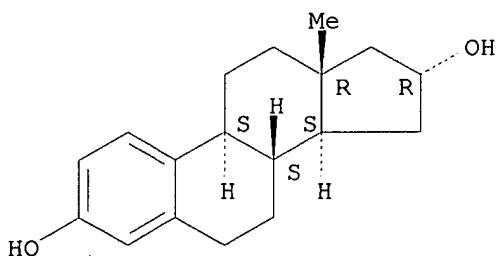
IT 1090-04-6

RL: BIOL (Biological study)
(estrone sulfotransferase inhibition by, kinetics of)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 60 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:543353 HCAPLUS

DOCUMENT NUMBER: 85:143353

TITLE: Preparation of tritiated substituted estratrienes

AUTHOR(S): Fraser, A. D.; Clark, S. J.; Wotiz, H. H.

CORPORATE SOURCE: Sch. Med., Boston Univ., Boston, MA, USA

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1976), 12(2), 213-18

CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1,3,5-(10)-Estratriene-3,6.beta.,17.beta., -3,16.beta.,17.beta.-, and 3,7.alpha.,17.beta.-triol with NBS gave the 2,4-dibromo derivs. which on catalytic tritiation gave the 2,4-tritiated compds. Similarly 1,3,5(10)-estratriene-3,11.beta.,17.beta.-triol-2,4-3H₂ and -3,16.alpha.-diol-2,4-3H₂ were prep'd. by direct iodination followed by catalytic tritiation. The T-labeled compds. had specific activities of 15.5-27.6 Ci/mmmole.

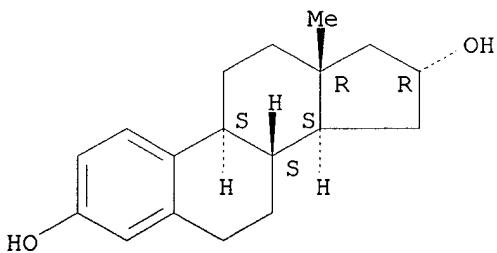
IT 1090-04-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



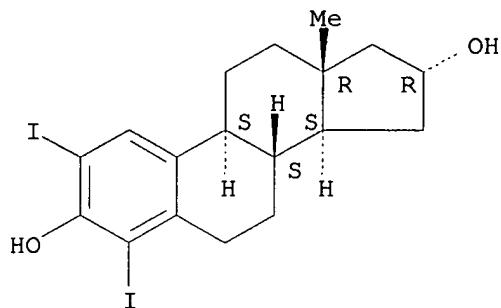
IT 60752-36-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and catalytic tritiation of)

RN 60752-36-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 2,4-diido-, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



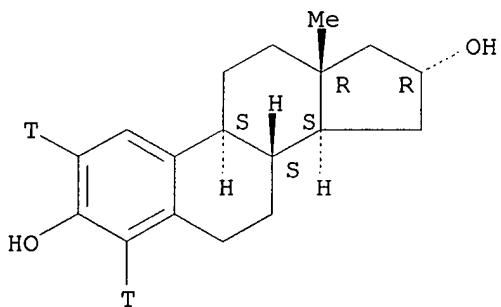
IT 60752-41-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)

RN 60752-41-2 HCPLUS

CN Estra-1,3,5(10)-triene-2,4-dien-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 61 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:99724 HCPLUS

DOCUMENT NUMBER: 84:99724

TITLE: Comparative specificity of three estradiol-binding proteins. Rat .alpha.-fetoprotein, rat liver 17.beta.-hydroxy steroid dehydrogenase, and anti-(estradiol-6-carboxymethyloxime-bovine serum albumin) antiserum

AUTHOR(S): Laurent, Chantal; De Lauzon, Solange; Cittanova, Nicole; Nunez, Emmanuel; Jayle, Max F.

CORPORATE SOURCE: CNRS, Paris, Fr.

SOURCE: Biochemical Journal (1975), 151(3), 513-18

CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Affinity studies with estradiol [50-28-2] and 30 other steroids indicated that rat .alpha.-fetoprotein, and rat liver microsomal 17.beta.-hydroxysteroid dehydrogenase [9028-61-9] recognized the edge of the steroid defined by C-4, C-6, C-8, and C-15 whereas artificially

induced anti-(estradiol-6-carboxymethyloxime-bovine serum albumin).gamma.-globulins recognized the opposite edge, defined by C-2, C-10, C-11, and C-17. Diethylstilbestrol [56-53-1] was recognized only by the 2 naturally occurring proteins.

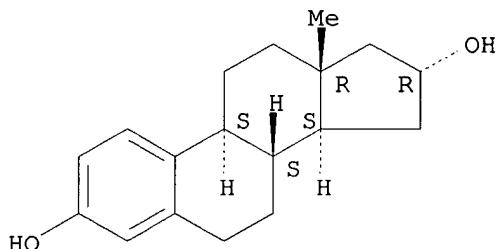
IT 1090-04-6

RL: BIOL (Biological study)
(estradiol-binding protein affinity for)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 62 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1974:534243 HCAPLUS

DOCUMENT NUMBER: 81:134243

TITLE: Steroid specificity of the estrogen receptor of human breast carcinoma

AUTHOR(S): Haehnel, Roland; Twaddle, Ella

CORPORATE SOURCE: King Edward Mem. Hosp. Women, Univ. West. Australia, Subiaco, Australia

SOURCE: Journal of Steroid Biochemistry (1974), 5(2), 119-22
CODEN: JSTBBK; ISSN: 0022-4731

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The specificity of the estrogen-receptor in human breast carcinoma was detd. by incubating the cytosol fraction with 17.beta.-estradiol-3H alone or in the presence of other steroids. If the steroid competed with the 17.beta.-estradiol-3H for binding sites on the receptor the binding of the 17.beta.-estradiol decreased. The structural requirements of the ligand for binding by the estrogen-receptor of breast carcinoma cytosol are the same as for that of human uterus cytosol. Highest affinity to the receptor is found if the steroid has a phenolic hydroxyl group on C-3 and an alc. hydroxyl group on C-17 in the .beta.-configuration. Variations of the functional groups with regard to nos., position, and state of oxidn. decrease the affinity for the receptor.

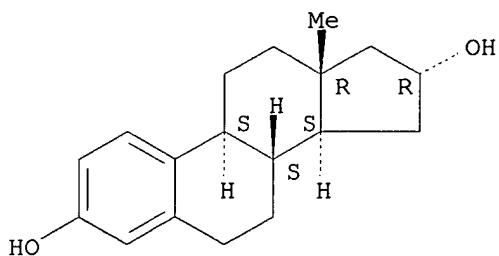
IT 1090-04-6

RL: PROC (Process)
(estrogen receptor site binding of, of mammary carcinoma)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 63 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1974:434965 HCAPLUS

DOCUMENT NUMBER: 81:34965

TITLE: Specificity studies on bovine adrenal estrogen sulfotransferase

AUTHOR(S): Rozhin, Jurij; Soderstrom, Robert L.; Brooks, Samuel C.

CORPORATE SOURCE: Michigan Cancer Found., Detroit, MI, USA

SOURCE: Journal of Biological Chemistry (1974), 249(7), 2079-87

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The substrate requirements for estrogen sulfotransferase were examined. Structural changes in all 4 rings of the estratriene nucleus affected sulfation. The Vmax of the reaction was increased from 1.4-3.2-fold over that of estrone by nitro groups at positions 2 or 4, or by the 6-keto function, while in the presence of a 2-amino group sulfation decreased to 1/3 and satn. of the A ring reduced sulfation to 0. The enzyme did not sulfate an OH in position 2 or 4 of estrogens but sulfated, with decreased efficiency, the phenolic-OH on 6-benzoyl naphthol, anthraquinone, fluorenes, diphenyl, and tetralin. Examn. of 59 structural variations showed the optimal sulfation of the phenolic-OH to require: (a) the presence of a lipophilic side chain (7 .ANG. long, para to the OH), and (b) in the estratriene nucleus, and O for H bonding to an area of the enzyme within 3.72 .ANG. above ring D.

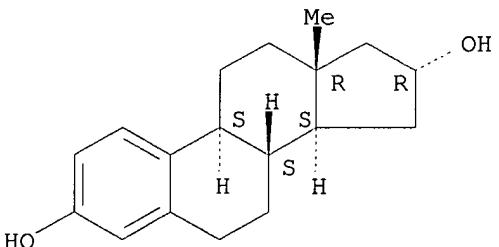
IT 1090-04-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfation of, enzymic)

RN 1090-04-6 HCAPLUS

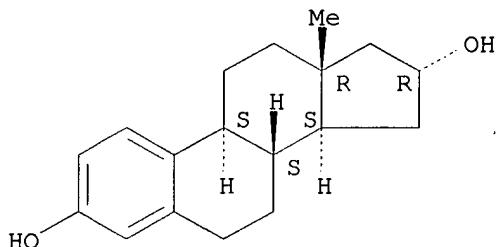
CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 64 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1973:511837 HCPLUS
 DOCUMENT NUMBER: 79:111837
 TITLE: Regulation of human placental steroid 3-sulfatase activity
 AUTHOR(S): Townsley, John D.
 CORPORATE SOURCE: Natl. Inst. Child Health Hum. Dev., Natl. Inst. Health, Bethesda, MD, USA
 SOURCE: Endocrinology (1973), 93(1), 172-81
 CODEN: ENDOAO; ISSN: 0013-7227
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The in vitro inhibitory activity of 129 endogenous and synthetic steroids on 17-oxo-5-androsten-3.beta.-yl sulfate hydrolysis by human term placental steroid 3-sulfatase [9025-62-1] was favored by planar .DELTA.5- or 5.alpha.-structures unsubstituted except for O functions at C-3 and C-20. Structure-activity data were compatible with binding of conjugated steroids to the enzyme via 3 sites, in addition to hydrophobic interactions. Alternative substrates, such as pregnenolone sulfate [1247-64-9], acting competitively, were the most potent inhibitors. Cumulative effects of other endogenous, competitive inhibitors, such as progesterone [57-83-0] and 17.beta.-estradiol [50-28-2], may reduce steroid sulfatase activity still further and contribute to the regulation of estrogen synthesis by the placenta.
 IT 1090-04-6
 RL: BIOL (Biological study)
 (steroid sulfatase inhibition by, in placenta)
 RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 65 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1973:505459 HCPLUS
 DOCUMENT NUMBER: 79:105459
 TITLE: Chromogenic reactions of steroids with strong acids.
 IV. Specificity of the Kober reaction
 AUTHOR(S): Kimura, Michiya; Kawata, Meiji; Akiyama, Kazuyuki;
 Harita, Kazuaki; Miura, Toshiaki
 CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1973), 21(8),
 1720-6
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB The structural requirements were investigated for the Kober reaction of steroidal mols. On the basis of the data given by 94 phenolic steroids and related substance, a compd. will give the pos. Kober reaction when a steroidal ring system, a phenolic ring A, double bond or O function in ring D, an angular Me group at C-13, and an angular H atom are present in its mol.

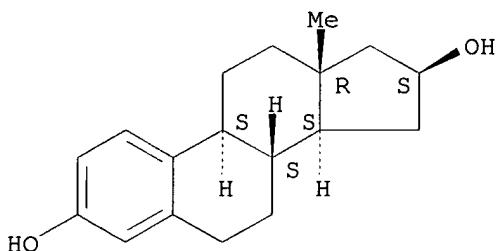
IT 1225-58-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(Kober reaction of, absorption spectra and)

RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 66 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1973:473903 HCPLUS

DOCUMENT NUMBER: 79:73903

TITLE: In vitro studies on the inhibition of pig liver steroid .DELTA.4-5.beta.-reductase activity by naturally occurring and synthetic estrogens

AUTHOR(S): Van Doorn, Edward J.; Clark, Albert F.

CORPORATE SOURCE: Kingston Gen. Hosp., Kingston, ON, Can.

SOURCE: Biochimica et Biophysica Acta (1973), 309(2), 254-62

CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal

LANGUAGE: English

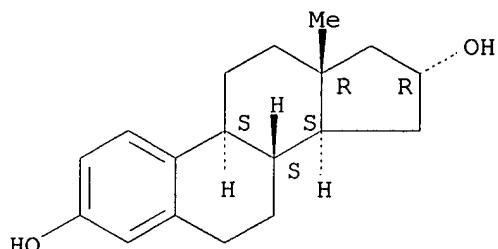
AB Of the naturally occurring estrogens studied, 2-hydroxyestradiol [362-05-0] and estradiol-3-sulfate [481-96-9] were the most potent inhibitors of testosterone [58-22-0] 5.beta.-redn. by a pig liver .DELTA.4-5.beta.-reductase prepn.; inhibitions of 35.2 and 37.0%, resp., were obsd. Among the synthetic estrogens, 16.alpha.-estradiol [1090-04-6], 17.alpha.-ethinyl-17.beta.-estradiol [57-63-6], and diethylstilbestrol [56-53-1] inhibited the redn. by 54.1, 55.6, and 86.8%, resp. The 5.beta.-redn. of cortisol [50-23-7] and aldosterone [52-39-1] was inhibited by ethinylestradiol to the same extent as that of testosterone. Three of the 4 members of the equine group of steroids studied exhibited inhibition; equilin [474-86-2] (56.3% inhibition) was the most active. Kinetic study indicated that diethylstilbestrol is a noncompetitive inhibitor of testosterone 5.beta.-redn.; the apparent Ki for this estrogen is 1.0 .tim. 10-6 M and the Km for testosterone .DELTA.4-5.beta.-reductase [9067-97-4] is 6.4 .tim. 10-6 M.

IT 1090-04-6

RL: BIOL (Biological study)
(steroid reductase inhibition by, in liver)

RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 67 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1973:427594 HCPLUS
 DOCUMENT NUMBER: 79:27594
 TITLE: Specificity of the estrogen receptor of human uterus
 AUTHOR(S): Haehnel, Roland; Twaddle, Ella; Ratajczak, Thomas
 CORPORATE SOURCE: Dep. Obstet. Gynaecol., King Edward Mem. Hosp.,
 Subiaco, Australia
 SOURCE: Journal of Steroid Biochemistry (1973), 4(1), 21-31
 CODEN: JSTBBK; ISSN: 0022-4731
 DOCUMENT TYPE: Journal
 LANGUAGE: English

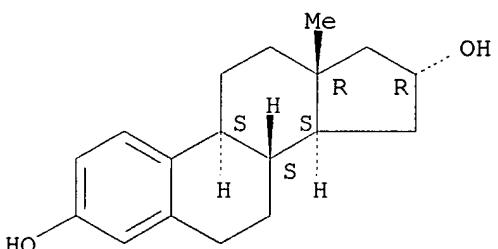
AB The estrogen receptor specificity of the human uterus was detd. from the relative abilities of various steroids to compete with 17.beta.-estradiol (I) [50-28-2] for receptor sites in the uterine cytosol fraction. Highest affinity for the receptor required a free phenolic OH group on C3 and an alc. group having the .beta.-configuration at C17, the former being particularly crit. Me groups at C1 or C4 decreased the affinity drastically, whereas the effect of a Me group at C2 was relatively slight. Addnl. O functions in ring D, addnl. substituents on ring A, and unsatn. in ring B decreased the affinity for the receptor, while the presence or absence of the angular Me group at C13 had no influence.

IT 1090-04-6

RL: BIOL (Biological study)
 (estradiol binding by uterus in response to)

RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 68 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1970:495274 HCAPLUS
 DOCUMENT NUMBER: 73:95274
 TITLE: Absorption and fluorescence spectra of phenolic steroids and their Kober chromophore
 AUTHOR(S): De Lauzon, Solange
 CORPORATE SOURCE: Lab. Chim. Biol., Fac. Med., Paris, Fr.
 SOURCE: Bulletin de la Societe de Chimie Biologique (1970), 52(2), 181-209
 CODEN: BSCIA3; ISSN: 0037-9042
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 AB A complete assignment was made of the absorption and fluorescence spectra of a no. of phenolic steroids and their derivs. and the results may be used to identify and det. each estrogen studied. The reaction of various derivs. which cannot be differentiated by the behavior of the Kober chromophore, or do not form a Kober chromophore, in H₂SO₄ and H₃PO₄ was used as an identification method. These derivs. included ketonic derivs. of estrone and estradiol, 16-hydroxy derivs. of estrone and their Et and Me ethers, and non-oxygenated C17 derivs. The Kober reaction was used as a detn. method for derivs. giving a characteristic absorption max., and the Ittrich modification allowed a sensitive anal. method to be developed for the steroid groups.

IT 1090-04-6 1225-58-7

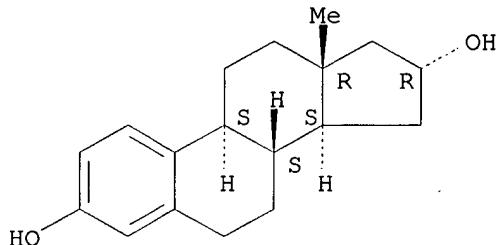
RL: PRP (Properties)

(fluorescence and visible spectra of, and its Kober chromogen)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

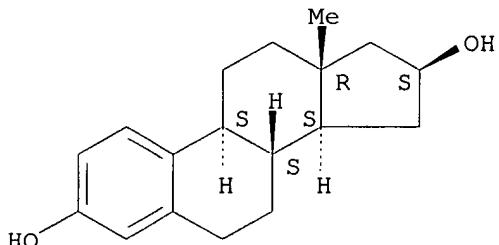
Absolute stereochemistry.

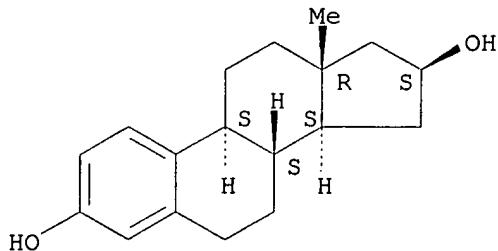


RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L5 ANSWER 69 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1970:452631 HCAPLUS

DOCUMENT NUMBER: 73:52631

TITLE: Steroid utilization by amphibian skin

AUTHOR(S): Ferguson, M. M.; McGadey, J.

CORPORATE SOURCE: Anat. Dep., Univ. Glasgow, Glasgow, UK

SOURCE: Histochemie (1970), 22(1), 36-8

CODEN: HICHAU; ISSN: 0018-2222

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The glands which secrete unpleasant tasting or toxic substances in amphibian dermis were investigated histochem. for hydroxysteroid dehydrogenase (I) activity to draw comparisons with mammalian sebaceous glands, which are known to utilize hydroxy steroids. Skin sections from frogs were incubated with 15 different steroids; serial sections were also stained with hematoxylin and eosin and by the periodic acid-Schiff (PAS) reaction to differentiate mucous glands. The frog skin contained at least 2 functional types of glands; one type was PAS-pos., while the second type, less common, was PAS-neg. but exhibited intense I activity. Tissue incubated with pregnenolone, dehydroepiandrosterone, 3. β .-hydroxyandrost-5-en-16-one 3-methyl ether, and 2. β .-hydroxyprogesterone exhibited no formazan deposits.

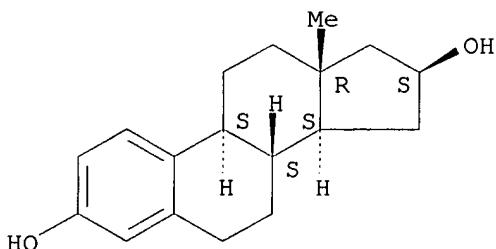
IT 1225-58-7

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by skin)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 70 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1970:3637 HCAPLUS

DOCUMENT NUMBER: 72:3637
 TITLE: 3,16.alpha.-Dihydroxy-16.beta.-ethynylestra-
 1,3,5(10)triene for treating hypercholesterolemia
 PATENT ASSIGNEE(S): Roussel-UCLAF
 SOURCE: Fr. M., 3 pp.
 CODEN: FMXXAJ
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 5099		19670626	FR	19660112

AB The title compd. (I) has a hypocholesterolemic effect and very low estrogenic activity. Thus, a mixt. of 260 ml tert-amyl alc. and 90 ml C6H6 was heated to 60.degree., 23.5 g K added slowly, the mixt. stirred 2 hr at 65.degree., 100 ml dioxane added at room temp., C2H2 passed into the mixt. for 2.5 hr, a soln. of 3.9 g 3-hydroxy-16-oxoestra-1,3,5(10)-triene in 120 ml dioxane added, the mixt. stirred 4 hr at 32-3.degree. in the presence of C2H2 stream, cooled, excess satd. NH4Cl added, the mixt. extd. with C6H6, and the org. phase worked up to give 528 mg I, m. 215.degree., [.alpha.]D 47.5.degree. (c 0.7, dioxane). Crude I was purified by SiO2 and Al2O3 chromatog. The daily dose for treating hypercholesterolemia is 5 mg/kg (female rat).

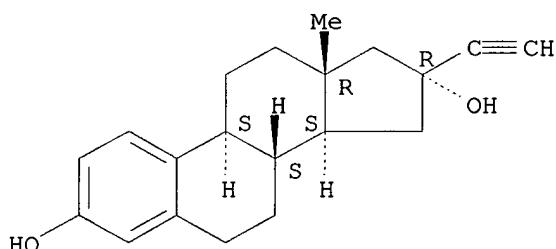
IT 24989-47-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); PREP (Preparation)
 (hypocholesterolemic effect of)

RN 24989-47-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 16-ethynyl-, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 71 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1969:74752 HCAPLUS
 DOCUMENT NUMBER: 70:74752
 TITLE: Comparative binding affinity of estrogens and its relation to estrogenic potency
 AUTHOR(S): Korenman, Stanley G.
 CORPORATE SOURCE: Harbor Gen. Hosp., Torrance, CA, USA
 SOURCE: Steroids (1969), 13(2), 163-77
 CODEN: STEDAM; ISSN: 0039-128X
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB The comparative affinity of steroidal and nonsteroidal estrogens for binding sites in rabbit uterine cytosol was detd. quant., using an in vitro assay system. With few exceptions, relative binding affinity paralleled uterotrophic activity. Binding affinity of steroids depended strongly on the phenolic OH and on substitutions in ring D. Addnl. substitutions of O functions or unsatn. of the estratriene nucleus were inhibitory. Synthetic estrogens competed and synthetic progestogens did not compete for cytosol binding sites. This binding assay may be used to det. estrogenic potency, though it must be borne in mind that binding does not distinguish between estrogens and competitive inhibitors.

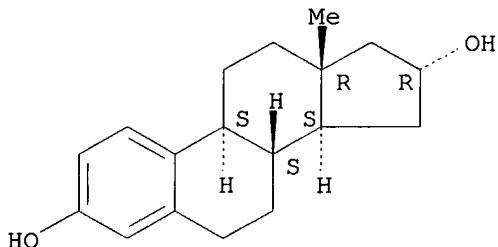
IT 1090-04-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(uterine binding activity of, mol. structure in relation to)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 72 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1969:9072 HCPLUS

DOCUMENT NUMBER: 70:9072

TITLE: Effect of various functional groups in the gas-liquid-chromatographic behavior of the estratriene nucleus

AUTHOR(S): Brooks, S. C.; Horn, L.

CORPORATE SOURCE: Sch. of Med., Wayne State Univ., Detroit, MI, USA

SOURCE: Analytical Biochemistry (1968), 25(1-3), 379-86

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The gas-liq. chromatographic behavior of 38 estrogens has been detd. on QF-1 and SE-30 columns and the contributions of the various functional groups to the retention characteristics of the estratriene nucleus were calcd. Equatorial hydroxyl groups had a longer retention effect than their axial epimers. Hydroxyl groups on the A or D rings of the estratriene nucleus increased the retention time more than did hydroxyls on the B or C rings.

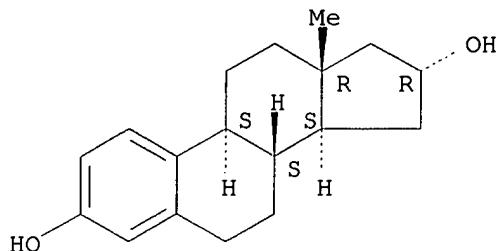
IT 1090-04-6

RL: PROC (Process)
(chromatog. of)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 73 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1968:464909 HCAPLUS

DOCUMENT NUMBER: 69:64909

TITLE: Stereospecificity of the uterine nuclear hormone receptors

AUTHOR(S): Brecher, Peter I.; Wotiz, Herbert H.

CORPORATE SOURCE: Sch. of Med., Boston Univ., Boston, MA, USA

SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1968), 128(2), 470-3

CODEN: PSEBAA; ISSN: 0037-9727

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Among 14 compds. (.ltoreq.5 .times. 10⁻² .mu.g./ml.) that significantly inhibited in vitro 17.beta.-estradiol binding by rat uterine nuclei, 17.beta.-estradiol, ethynodiol, hexestrol, and diethylstilbestrol were the most effective; the least effective compds. of this group included estriol, 17-hydroxyestrone, and 16-ketoestrone. Thirteen other compds. including 1,3,5(10),16-estratetraen-3-ol, 2-hydroxyestrone, and testosterone were ineffective as inhibitors. All of these were compds. not possessing the estratriene nucleus of the steroid estrogens, but with modifications in ring A. Specificity may involve any or all of the receptors and transferring enzyme systems. Moreover, specificity may vary somewhat between macromols.

IT 1090-04-6

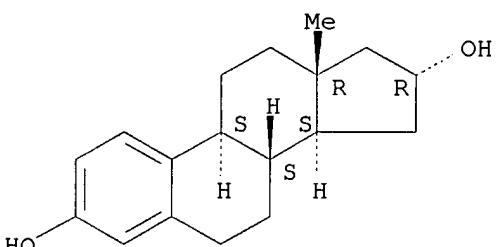
RL: BIOL (Biological study)

(estradiol binding by uterine receptor inhibition by)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

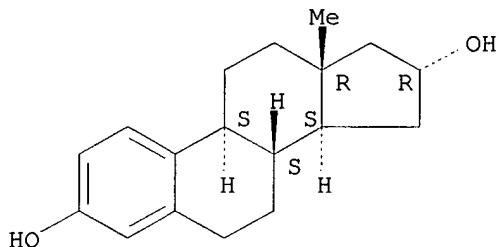
Absolute stereochemistry.



L5 ANSWER 74 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1968:63476 HCPLUS
 DOCUMENT NUMBER: 68:63476
 TITLE: Crystal data for some estrone-related compounds. III.
 AUTHOR(S): Ohrt, Jean M.; Haner, Barbara A.; Norton, Dorita A.
 CORPORATE SOURCE: Roswell Park Mem. Inst., Buffalo, NY, USA
 SOURCE: Acta Crystallographica (1967), 23(6), 1100
 CODEN: ACCRA9; ISSN: 0365-110X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The lattice consts. of 10 estrone related compds. were detd. by x-ray diffraction [compd., space group, a, b, c, .alpha., .beta., .gamma., Z given]: 3-methoxy-19-norandrosta-2(3),5(10)-dien-17.beta.-ol, P21, 7.114, 36.573, 6.963 A., -, 100.60.degree., -, 4; estron-17-enol acetate 3-methyl ether, P212121, 9.105, 32.300, 6.115 A., -, -, -, 4; estra-1,3,5(10)-triene-3,17.beta.-diol diacetate, P212121, 17.698, 26.799, 8.173 A., -, -, -, 8; estra-1,3,5(10)-trien-3-ol-16,17-dione 16-oxime, P212121, 12.180, 16.183, 7.824 A., -, -, -, 4; estriol triacetate, P21, 18.704, 8.678, 13.746 A., -, 91.30.degree., -, 4; 17.alpha.-ethylestradiol 3-methyl ether, P212121, 15.296, 39.316, 6.552 A., -, -, -, 8; 1-methyl-estrone, P212121, 11.980, 12.482, 10.640 A., -, -, -, 4; estriol methyl ether, (P31, P32), 7.011, -, 57.076 A., -, -, 120.00.degree., 6; 16.alpha.-estradiol, P21, 9.288, 23.317, 7.388 A., -, 109.03.degree., -, 4; D-equilenin, P212121, 7.480, 25.528, 7.279 A., -, -, -, 4.

IT 1090-04-6
 RL: PRP (Properties)
 (crystal structure of)
 RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 75 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1967:440551 HCPLUS
 DOCUMENT NUMBER: 67:40551
 TITLE: Modified procedure for estimating estrogens in urine
 AUTHOR(S): Jones, Patricia Halbert; Erb, Ralph E.
 CORPORATE SOURCE: Purdue Univ., Lafayette, IN, USA
 SOURCE: Journal of Dairy Science (1967), 50(5), 772-4
 CODEN: JDSCAE; ISSN: 0022-0302
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Estn. by gas-liq. chromatog. (GLC) was combined with sepn. and quant. steps outlined by Mellin, et al. (CA 63: 7285c). Thirteen steroid standards and their trimethylsilyl ethers derivs. were chromatographed on

0.318-cm. diam. columns, packed with 1.83-m. lengths of SE-30, and 3.66 m. of a 1:1 mixt. of SE 30 and XE-60 on 80-100 mesh Gas-Chrom Q. The instrument was equipped with a flame-ionization detector coupled to an Isothermal temp. control. Operating conditions were as follows: oven 250.degree., injector 295.degree., H and N flow rates 30 ml./min. each, injected amts. 1 .mu.l. of soln. contg. 2 .gamma. of steroids. The retention times, relative to 5.alpha.-cholestane, on the 2 columns were detd. The min. detectable of keto steroid is 0.05 .gamma., and the min. amt. of estradiol 0.01 .gamma..

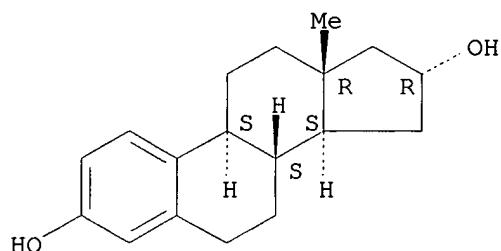
IT 1090-04-6

RL: PROC (Process)
(chromatog. of)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 76 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1967:112529 HCPLUS

DOCUMENT NUMBER: 66:112529

TITLE: Chromogenic steroid reactions induced by silica in dilute sulfuric acid, useful for detection of steroids on thin-layer chromatoplates without heating, and a note on the specificity of the so-called Oertel, Allen, and Jensen reactions

AUTHOR(S): Carstensen, Hans

CORPORATE SOURCE: Univ. Uppsala, Uppsala, Swed.

SOURCE: Journal European des Steroides (1966), 1(3), 233-86
CODEN: JEPSBL; ISSN: 0531-4186

DOCUMENT TYPE: Journal

LANGUAGE: English

AB It was established that H_2SO_4 -EtOH reactions such as the one proposed by Oertel (CA 53, 9338g), for .DELTA.5-3.beta.-hydroxy steroids of the C21 and C19 series are also given by .DELTA.4-3.alpha.- or .DELTA.4-3.beta.-hydroxy steroids as well as by certain satd. 3-hydroxy steroids and by pregn-5-ene-3,20-dione but not by androst-5-ene-3,17-dione. When silica gel chromatoplates were sprayed with these reagents, the steroids of the same groups formed a bright pink color that had varying stability but had the advantage of being rapidly formed without heating which enabled its use for the location of standard steroids that were run in parallel to exts. For the .DELTA.5- or .DELTA.4-unsatd. steroids mentioned silica sol induced a transformation of max. absorbancy when they were treated with H_2SO_4 -H₂O or H_2SO_4 -EtOH reagents so that the peak at 405-408 m.mu. shifted to 485-488 m.mu.. This shift was often slow and incomplete depending upon structural features of the steroids. It was

inferred that the activated form of the steroid formed an auxochromic complex with silica. When certain org. solvents (Et₂O, EtOH, EtOAc) were afterwards added to the reaction mixt. a further transformation of absorption max. was caused with the appearance of a peak at 520-50 m.m.u.. This corresponded to the pink color observed on the chromatoplates. After a while there was a further shift to longer wavelengths with max. around 600 m.m.u. and a violet-blue color. Heating at 55-60.degree. followed by diln. with EtOH or Et₂O gave an increased absorbancy at 600 m.m.u. not only for .DELTA.5-3.beta.-hydroxy C₁₉ steroids as found by Allen (A., et al., CA 47, 1763c) and by Jensen (Acta Endocrinol. 4, 140(1950)) but also for .DELTA.4-3-hydroxy and .DELTA.4-3-keto C₁₉ steroids, while .DELTA.5-3.beta.-hydroxy C₂₁ steroids failed to give this chromogen. Color reactions given by specific steroids are discussed in detail. 22 references.

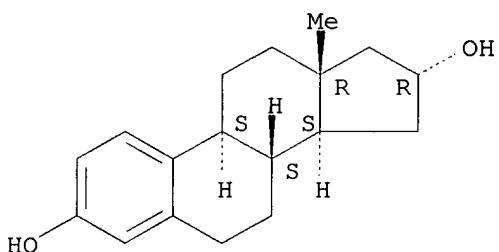
IT 1090-04-6

RL: BIOL (Biological study)
(color reaction with sulfuric acid and its spectrum)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 77 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1966:88121 HCPLUS

DOCUMENT NUMBER: 64:88121

ORIGINAL REFERENCE NO.: 64:16601d-e

TITLE: Response of steroids to H₂SO₄ in thin-layer chromatography

AUTHOR(S): Heftmann, Erich; Ko, Shui Tze; Bennett, Raymond D.

CORPORATE SOURCE: Western Regional Res. Lab., Albany, CA

SOURCE: Journal of Chromatography (1966), 21(3), 490-4

CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The steroids were dissolved in CH₂Cl₂ and 4 .gamma. of each compd. was spotted on a silica gel G layer, 250 .mu. thick. The spot area was .apprx.20 mm.² The plates were sprayed with 50% H₂SO₄ and heated on a hot plate at a surface temp. of 78.degree.. The time required for the initial appearance of a color, the initial color in daylight, the color after heating for 10 min., and the color in long wave (366 m.m.u.) uv light were recorded. Results for 141 representatives of various classes of steroids are tabulated.

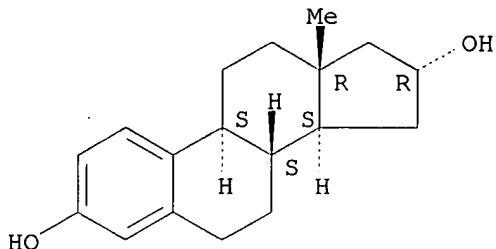
IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.alpha.-diol

(color reaction with H₂SO₄ on thin-layer chromatograms)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 78 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1965:498740 HCAPLUS

DOCUMENT NUMBER: 63:98740

ORIGINAL REFERENCE NO.: 63:18220d-h

TITLE: A-Nor-B-homo steroids

PATENT ASSIGNEE(S): CIBA Ltd.

SOURCE: 13 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6412652		19650503	NL	

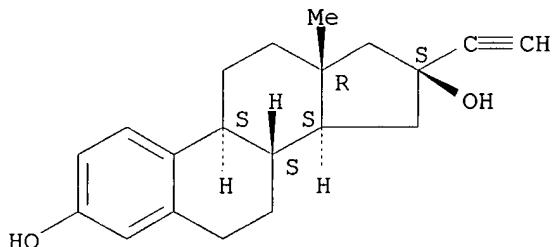
PRIORITY APPLN. INFO.: CH 19631101

AB A series of 3,6-dioxo-A-nor-B-homo steroids was prep'd. by treating 11-unsubstituted or 11-hydroxy-4-sulfonyloxy-5-hydroxysteroid 3-ketals with tert-BuOK. Testosterone acetate (I) (3.7 g.), 200 mg. adipic acid, 100 cc. C6H6, and 25 cc. (CH2OH)2 refluxed 46 hrs. with the azeotropic removal of H2O, and the crude product (3.97 g.) chromatographed on Al2O3 yielded 2.2 g. 3,3-ethylenedioxy-17.beta.-acetoxy-4-androstene (II), m. 149-51.degree. (Me2CO-petroleum ether), [.alpha.]D 85.degree. (c 0.83, CHCl3). II (1.1 g.) in 10 cc. C5H5N treated 2 hrs. at 20.degree. and 12 hrs. at -30.degree. with 2 cc. MeSO2Cl, and the crude product (950 mg.) chromatographed on silica gel yielded 60 mg. I and 702 mg. 4-mesyloxy-5-hydroxyandrostan-17.beta.-ol-3-one 17-acetate, m. 190-1.degree. (decompn.) (Me2CO-petroleum ether), [.alpha.]D 25.degree. (c 0.69, CHCl3); a 50-mg. portion in 50 cc. C6H6 and 20 cc. (CH2OH)2 refluxed 5 hrs. with 50 mg. p-MeC6H4SO3H with the azeotropic removal of H2O yielded 40 mg. 3,3-ethylenedioxy-17.beta.-acetoxy-4-mesyloxy-5-hydroxyandrostane (III), m. about 180.degree. (Me2CO-petroleum ether), which hydrolyzed with K2CO3-MeOH gave the 17.beta.-OH analog (IV) of III. IV (50 mg.) and 50 mg. tert-BuOK in 50 cc. tert-BuOH refluxed overnight yielded 30 mg. A-nor-B-homoandrostan-17.beta.-ol-3,6-dione (V), m. 117-18.degree. (CH2Cl2hexane). 17.alpha.-Me deriv. of I was converted similarly to the 17.alpha.-Me deriv. of V, m. 168-70.degree., [.alpha.]D 34.degree. (c 0.92, CHCl3). I (3 g.) in 100 cc. Et2O stirred 24 hrs. at room temp. with 100 mg. OsO4 and 6 cc. 30% H2O2, treated with an addnl. 6 cc. 30% H2O2 and 100 mg. OsO4, and stirred 6 days at room temp. yielded 3.39 g. 17.beta.-acetoxyandrostane-4,5-diol-3-one (VI), m. 169.degree.

(Me₂CO-petroleum ether), [α]_D 27.° (c 0.64, CHCl₃). VI (1.14 g.) in 10 cc. C₅H₅N treated 2.5 hrs. at room temp. with 2 cc. MesO₂Cl yielded 1.12 g. 4-methanesulfonate of VI, m. 190.° (Me₂CO-petroleum ether), [α]_D 25.° (c 0.69, CHCl₃). By the general method were prep'd. the following compds. (m.p. given): A-nor-B-homopregn-20-ol-3,6-dione, 117-18.°; A-nor-B-homocholestane-3,6-dione-, 7.α., 17.α.-dimethyl-A-nor-B-homoestran-17.-β.-ol-3,6-dione, 168-9.°; 7.α., 17.α.-dimethyl-A-nor-B-homoandrostan-17.β.-ol-3,6-dione, 162-3.°; 17.α.-ethynyl-A-nor-B-homoestran-17.β.-ol-3,6-dione, 156-8.°; 17.α.-ethynyl-A-nor-B-homoestran-17.β.-ol-3,6-dione, 166-8.°; 17,20:20,21-bis(methylenedioxy) deriv. of A-nor-B-homopregnane-11.β., 17.α., 21-triol-3,6,20-trione (VII) 192-4.° (which hydrolyzed gave VII, m. 142-4.°). The new 19-norandrostan derivatives show anabolic and antiovulation activity, the 19-norpregnane derivs. progestational and antiinflammatory activity.

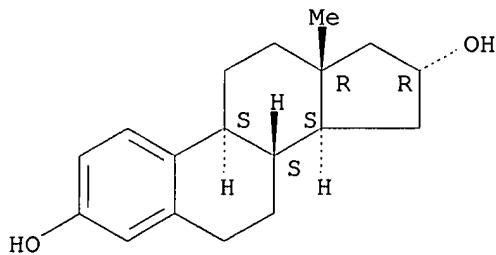
IT 4138-97-0, Estra-1,3,5(10)-triene-3,16.β.-diol, 16-ethynyl-
(prepn. of)
RN 4138-97-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,16.β.-diol, 16-ethynyl- (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 79 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1965:55819 HCAPLUS
 DOCUMENT NUMBER: 62:55819
 ORIGINAL REFERENCE NO.: 62:9889g-h
 TITLE: X-ray diffraction powder data for steroids. V
 AUTHOR(S): Parsons, Jonathan; Wong, S. T.; Beher, William T.
 SOURCE: Henry Ford Hospital Medical Bulletin (1964), 12(4), 459-75
 CODEN: HFHMAF; ISSN: 0096-1868
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB cf. CA 58, 14031b; 61, 1332f.
 IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.α.-diol
 (x-ray diffraction powder data for)
 RN 1090-04-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.α.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 80 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1965:10380 HCPLUS

DOCUMENT NUMBER: 62:10380

ORIGINAL REFERENCE NO.: 62:1938e-f

TITLE: A search for inhibitors of prostate growth stimulators

AUTHOR(S): Tesar, Charles; Scott, William Wallace

CORPORATE SOURCE: Johns Hopkins Hosp., Baltimore, MD

SOURCE: Investigative Urology (1964), 1(5), 482-98

CODEN: INURAQ; ISSN: 0021-0005

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Wistar rats received 0.4 mg. testosterone propionate (I) subcutaneously every other day for 8 days following castration. Test compds. were given at 0.5, 1, and 2 mg. every other day for 7 days, with or without 0.4 mg. I in castrate and noncastrates, resp. Within 48 hrs. of the 7th (final) injection, animals were sacrificed with CHCl₃, and the prostate wt. to body wt. ratio, and the prostate wt. index were detd. The greatest prostate growth inhibitor was 17. β -estradiol, and some weak inhibition was seen with 6. α -methyl-4-pregnene-3,20-dione-17. α -ol acetate, androstane-3,17-dione, and 2. α -methyl-4-estren-17. β -ol-3-one, the inhibitory effect being seen only in intact rats, and not in castrates, for all 52 compds. tested.

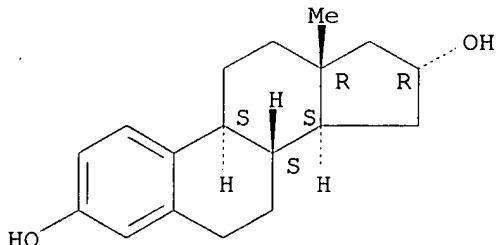
IT 1090-04-6, Estra-1,3,5(10)-triene-3,16. α -diol

1225-58-7, Estra-1,3,5(10)-triene-3,16. β -diol
(as prostate growth inhibitor)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. α .)- (9CI) (CA INDEX NAME)

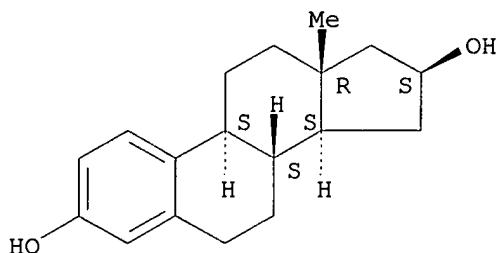
Absolute stereochemistry.



RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 81 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1964:91104 HCAPLUS

DOCUMENT NUMBER: 60:91104

ORIGINAL REFERENCE NO.: 60:15942c-e

TITLE: Hydration of unsaturated steroids by the brown hydroboration reaction. I. Monounsaturated steroids

AUTHOR(S): Nussbaum, Manasse; Mazur, Yehuda; Sondheimer, Franz

CORPORATE SOURCE: Weizmann Inst. Sci., Rehovoth, Israel

SOURCE: Journal of Organic Chemistry (1964), 29(5), 1120-31

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

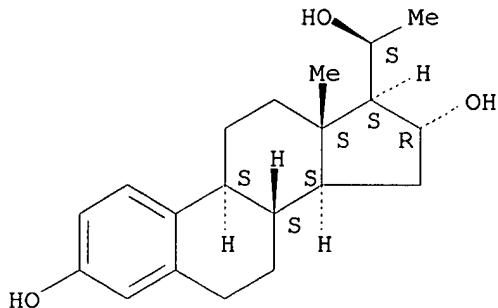
AB A wide variety of monounsatd. steroids was subjected to hydration by the Brown method (involving hydroboration and subsequent oxidn. with alk. H₂O₂), in order to investigate the scope and steric course of the reaction. The hydroboration step was carried out either by means of LiAlH₄ and BF₃ in situ or alternatively by passing in diborane gas. Nearly all of the unsatd. steroids studied could be hydrated successfully by this method, the only exceptions noted being the highly hindered .delta.7-, .delta.9(11)-5.beta.-, and .delta.8(14)-ethylenes. Hydration in all cases proceeded by overall cis addn. of the elements of H₂O, predominantly from the less hindered side (usually the .alpha. side) of the mol. In the case of steroids contg. 1,2-disubstituted double bonds, approx. equal amts. of both possible positionally isomeric alcs. were obtained, while steroidal trisubstituted ethylenes gave only the secondary alcs. (anti-Markovnikov addn.). Hydroboration of certain 1,2-disubstituted steroidal ethylenes with bis(3-methyl-2-butyl)borane (disiamylborane) was also investigated, and it was found that in the case of 5.alpha.-cholest-1-ene this reagent resulted in the formation of only 5.alpha.-cholest-2.alpha.-ol.

IT 104073-24-7, 19-Norpregna-1,3,5(10)-triene-3,16.alpha.,20.alpha.-triol
(prepn. of)

RN 104073-24-7 HCAPLUS

CN 19-Norpregna-1,3,5(10)-triene-3,16.alpha.,20.alpha.-triol (7CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 82 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1962:464495 HCAPLUS

DOCUMENT NUMBER: 57:64495

ORIGINAL REFERENCE NO.: 57:12883f-h

TITLE: The steroid specificity of the 17. β -hydroxysteroid dehydrogenase of human placenta

AUTHOR(S): Adams, Julia A.; Jarabak, Joseph; Talalay, Paul

CORPORATE SOURCE: Univ. of Chicago

SOURCE: Journal of Biological Chemistry (1962), 237, 3069-73

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

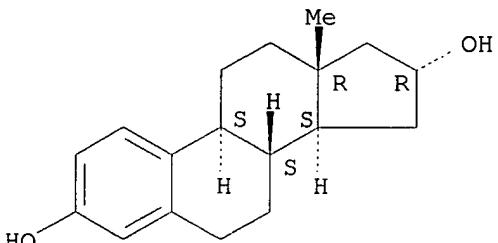
AB Studies have been made on the steroid specificity and the effects of diethylstilbestrol on highly purified preps. of the 17. β -hydroxysteroid dehydrogenase of human placenta, both in its dehydrogenase and its transhydrogenase functions. Diethylstilbestrol is a competitive inhibitor of the transhydrogenase function of this enzyme and does not, at any concn., stimulate the reaction in the presence or absence of added 17. β -estradiol. Various aromatic and nonaromatic 17. β -hydroxy steroids of the C18 and C,19 series can serve as substrates for the dehydrogenase reaction. There is a close correlation between steroids that undergo oxidn. and those that mediate the transhydrogenase function of this enzyme.

IT 1090-04-6, Estra-1,3,5(10)-triene-3,16. α -diol
(oxidn. by 17. β -hydroxy steroid dehydrogenase)

RN 1090-04-6 HCAPLUS

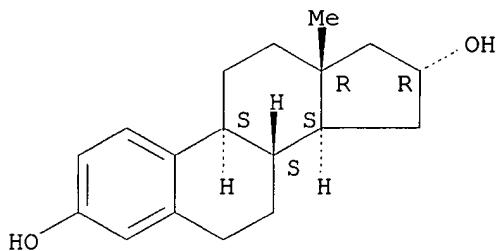
CN Estra-1,3,5(10)-triene-3,16-diol, (16. α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



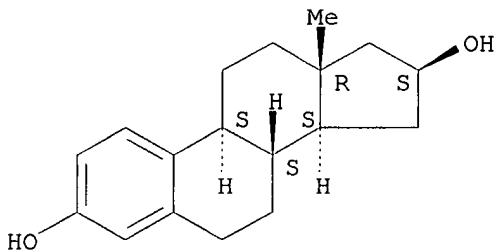
L5 ANSWER 83 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1960:98911 HCAPLUS
 DOCUMENT NUMBER: 54:98911
 ORIGINAL REFERENCE NO.: 54:18799c-d
 TITLE: Cytostatic activities of steroidal estrogens against zebra-fish embryos
 AUTHOR(S): Jones, Roy W.; Rhone, James R.; Huffman, Max N.
 CORPORATE SOURCE: Oklahoma State Univ., Stillwater
 SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1960), 104, 190-1
 CODEN: PSEBAA; ISSN: 0037-9727
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. CA 52, 3171c. The cytostatic effects of 14 steroidal estrogens (named) and the 3-Me and 3-Et ethers of each were tested on embryos of zebra-fish (*Brachydanio rerio*) as test object. Many were inactive in the concns. used. Most active was 17-dihydro-17 β -equilin 3-ethyl ether (effective at 0.5 p.p.m.). There was no relation whatever between estrogenic hormone potency and cytostatic potency.
 IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.alpha.-diol
 1225-58-7, Estra-1,3,5(10)-triene-3,16 β .-diol
 (as cell-division inhibitor)
 RN 1090-04-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 1225-58-7 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16 β .)- (9CI) (CA INDEX NAME)

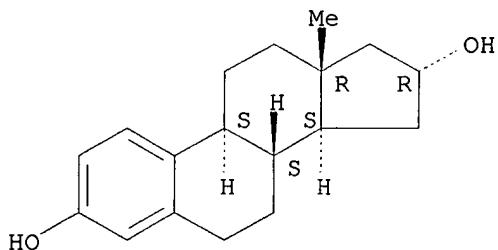
Absolute stereochemistry.



L5 ANSWER 84 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1960:98910 HCAPLUS

DOCUMENT NUMBER: 54:98910
 ORIGINAL REFERENCE NO.: 54:18799b-c
 TITLE: Accumulation of strontium-90 and calcium-45 by fresh water fishes
 AUTHOR(S): Rosenthal, Harold L.
 CORPORATE SOURCE: Washington Univ., St. Louis, MO
 SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1960), 104, 88-91
 CODEN: PSEBAA; ISSN: 0037-9727
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. CA 52, 3179f, 8393i. An extension of previous work, showing influence of variations in concn. on uptake, and the influence of Na+. At low concns. of Na+ Danio, Tanichthys, and Lebistes all discriminate against Sr90 as compared with Ca45 by factors of 0.921-0.964. As Na+ concn. is increased the discrimination becomes less and is essentially absent at concns. greater than 20 mM.
 IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.alpha.-diol
 (as cell-division inhibitor)
 RN 1090-04-6 HCPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 85 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1960:74827 HCPLUS
 DOCUMENT NUMBER: 54:74827
 ORIGINAL REFERENCE NO.: 54:14309a-e
 TITLE: 16.alpha.-Hydroxysteroids
 PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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GB 823955		19591118	GB	

AB The title compds., their ethers and esters were prep'd. by heating an arenesulfonate of the corresponding 16.beta.-ol with an alkali metal lower alkanoate in the corresponding alkanoic acid and sapong. the resulting 16.alpha.-acylate. Thus, 4.4 g. p-MeC₆H₄SO₂Cl added to a soln. of 1 g. 1,3,5(10)-estratriene-3,16.beta.-diol in 28 ml. dry C₅H₅N at 0.degree., the mixt. kept 2 days, dild. with ice H₂O contg. 10% NaCl, left 24 hrs. at 5.degree., extd. with Et₂O, the exts. washed, the washings extd. with Et₂O

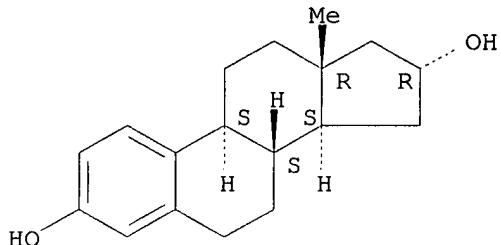
and the combined exts. evapd. gave 1.9 g. crude 3,16.beta.-ditosylate, which refluxed 1 hr. with 4.8 g. fused NaOAc in 92 ml. AcOH, the mixt. cooled and dild. with ice H₂O contg. 10% NaCl, after 24 hrs. the ppt. sepd., dried and refluxed 1 hr. with 60 ml. 2.5N KOH in 200 ml. MeOH, the MeOH distd., 100 ml. H₂O, then 10 ml. concd. HCl added, the pH adjusted to 5-6, the ppt. sepd., dried at 40.degree. and crystd. from Me₂CO-hexane then aq. MeOH gave 0.55 g. 3,16.alpha.-estradiol (I), m. 213-15.degree., raised to 224-4.5.degree., [.alpha.]₂₅D 85.degree. (c 0.76, 95% EtOH), after purification via its 3,16.alpha.-diacetate, m. 116-17.degree.. Benzoylation of I in 0.5N NaOH gave the 3-monobenzoate, m. 179.5-81.0.degree.; benzoylation in C₅H₅N gave the 3,16-dibenzoate, m. 130.5-1.5.degree.. Similarly, 118 mg. 3-methoxyestra-1,3,5(10)-trien-16.beta.-ol gave 38 mg. estradiol 16.alpha.-acetate 3-methyl ether, m. 123-3.5.degree.; 575 mg. androstan-3.beta.-ol-16-one dissolved in 300 ml. refluxing MeOH, cooled, 0.39 g. NaBH₄ added, the soln. swirled 1 hr., 4 ml. 50% AcOH added, the soln. concd. to 100 ml. and 100 ml. ice H₂O added yielded 550 mg. 3.beta.-benzoyloxyandrostan-16.beta.-ol (II), m. 168-9.degree.; 400 mg. II epimerized as above gave androstane-3.beta.,16.alpha.-diol, m. 187.5-88.degree., [.alpha.]₂₅D -4.degree. (c 0.777, 95% EtOH), which with Ac₂O in C₅H₅N gave the diacetate, m. 174-4.5.degree. [.alpha.]₂₃D -26.degree. (c 0.963, CHCl₃). Other starting materials are equilenin-16-one and 5-isoandrosterone. I displays considerable estrogenic activity, in contrast to its 16.beta. epimer.

IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.alpha.-diol
(effect on mammary neoplasm and phosphatases in)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



(esters

L5 ANSWER 86 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1959:17432 HCPLUS
DOCUMENT NUMBER: 53:17432
ORIGINAL REFERENCE NO.: 53:3276g-i,3277a-f
TITLE: Synthesis of 1,3,5(10)-estratriene-3,16.beta.,17.alpha.-triol
AUTHOR(S): Fishman, Jack; Biggerstaff, Warren R.
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Research, New York,
NY
SOURCE: Journal of Organic Chemistry (1958), 23, 1190-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Prepn. of 1,3,5(10)-estratriene-3,16.beta.,17.alpha.-triol (I) is

described. The 16.alpha.- (II) and 16.alpha.-bromo epimers (III) of estrone were also prep'd. and some of their reactions studied. Of the 4 possible estriols isomeric at C-16 and C-17 only 3 are known. The present authors undertook the prepn. of the remaining isomer, I. Estrone enol diacetate (1 g.) in CCl_4 contg. some K_2CO_3 was treated with 1 equiv. of Br in CCl_4 and the mixt. worked up to give 700 mg. 16.alpha.-bromoestrone acetate (IV), m. 169-71.degree. (MeOH), [α]_{24D} 119.degree. (CHCl_3). IV (0.3 g.) in 4% alc. H_2SO_4 left 20 hrs. at room temp., dild. with H_2O , and extd. with CHCl_3 gave 243 mg. II, needles, m. 225-8.degree. (C_6H_6), [α]_{24D} 120.degree. (CHCl_3). Acetylation of II with Ac_2O and $\text{C}_5\text{H}_5\text{N}$ regenerated IV. IV (0.5 g.) in a min. amt. of 1:1 C_6H_6 -ligroine was absorbed on Al_2O_3 , left overnight on the column and eluted with first 3:2 and then 4:1 C_6H_6 -ligroine, and the fractions combined on the basis of m.p. The first 5 fractions gave on crystn. 0.23 g. pure IV. Fractions 6-10 were mixts., and fractions 10-14 gave 47 mg. 16.beta.-bromoestrone acetate (V), needles, m. 170-3.degree. (MeOH), [α]_{25D} 156.degree. (CHCl_3). Subsequent fractions eluted from the column with more polar solvents proved to be a mixt. of the hydrolyzed II and III. A mixed m.p. of V with IV showed a depression of 40.degree.; the infrared spectra of II and III in CS_2 were different in the 1400-650 cm^{-1} , but there was no difference in the position of the CO band at 1758 cm^{-1} . Paper chromatography in several systems failed to sep. the 2 isomers. Room temp. hydrolysis of V 20 hrs. with 4% alc. H_2SO_4 gave free III, needles, m. 224-7.degree. (sublimation) (C_6H_6). An analytical sample of III m. 225-8.degree., [α]_{24D} 154.degree. (CHCl_3). III could be obtained by refluxing IV with 4% alc. H_2SO_4 overnight; the resultant mixt. was predominantly III which was purified by fractional crystn. Acetylation of III gave V. IV (1 g.) stirred 2 hrs. at 0.degree. with excess LiAlH_4 in anhyd. Et_2O , the excess reagent destroyed with H_2O and acidified with dil. HCl , and the org. phase evapd. gave 0.78 g. gum. Without purification, the material refluxed 4 hrs. with 5% alc. KOH , dild. with H_2O , extd. with CHCl_3 , and chromatographed on Al_2O_3 gave 0.24 g. 16.beta.,17.beta.-epoxy-1,3,5(10)-estratrien-3-ol (VI), m. 200-4.degree. (C_6H_6 -ligroine), [α]_{25D} 119.degree. (CHCl_3), and 92 mg. estrone. The structure of VI was established by reduction with LiAlH_4 to give 16.beta.-estradiol (VII), identical with a specimen prep'd. from 1,3,5(10)-estratrien-16-one by NaBH_4 reduction. VII m. 224-6.degree.. V (150 mg.) reduced under identical conditions with LiAlH_4 followed by heating with alkali gave 94 mg. estrone. No 16.alpha.,17.alpha.-oxide was isolated. VI (0.3 g.) in 30 cc. AcOH refluxed 4 hrs., evapd., refluxed 1.5 hrs. with 6% alc. KOH , dild., acidified, and extd. with CHCl_3 gave 0.3 g. solid which was chromatographed on Al_2O_3 to give 124 mg. I, m. 248-50.degree. (C_6H_6 - MeOH), [α]_{25D} 61.degree. (alc.). The subsequent fractions eluted weighed 64 mg. and proved to be the other trans isomer, 1,3,5(10)-estratriene-3,16.beta.,17.alpha.-triol (VIII). The infrared spectrum of I in KBr showed differences from the other 3 estriol isomers. Paper chromatography in C_6H_6 - MeOH - H_2O - EtOAc system sepd. I from its isomers. I was less polar than VIII but considerably more polar than the 2 cis triols in the solvent system used. 1,3,5(10),16-Estratetraen-3-ol benzoate (100 mg.), m. 161-6.degree., in Et_2O treated with BzO_2H gave 111 mg. crude 16.alpha.,17.alpha.-epoxy-1,3,5(10)-estratrien-3-ol benzoate. Without further purification this material was refluxed 2 hrs. with 3 cc. AcOH under N, the AcOH removed, and the residue refluxed 1.5 hrs. in 8% alc. KOH to give 73 mg. yellow solid, which, decolorized and crystd., gave 23 mg. solid which was chromatographed on silica to give 12 mg. I. These results confirm the assignment of the Br orientation in II and III and also support the previous finding (C.A. 52, 5445b) that a

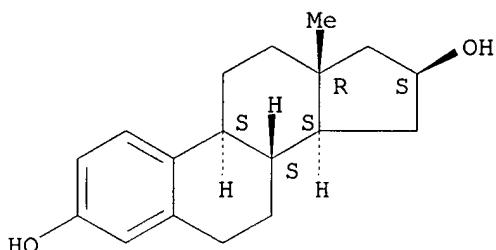
16. β -substituent results in the stereospecific β -reduction of the 17-one while a 16. α -substituent makes the reduction only stereoselective, with about 10-15% of α -reduction. The pharmacol. effects are being investigated.

IT 1225-58-7, Estra-1,3,5(10)(triene-3,16. β -diol
(prep. of)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 87 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1958:93818 HCAPLUS

DOCUMENT NUMBER: 52:93818

ORIGINAL REFERENCE NO.: 52:16548d-f

TITLE: Comparative ability of some steroids and their esters to enhance the renal β -glucuronidase activity of mice

AUTHOR(S): Fishman, Wm. H.; Lipkind, J. B.

CORPORATE SOURCE: Tufts Univ. School of Med., Boston, MA

SOURCE: Journal of Biological Chemistry (1958), 232, 729-36

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 50, 17081h. The mouse renal β -glucuronidase response permits a more reliable estimate of the potency of testosterone esters. A dose-response curve in which greatly reduced amts. of steroid were used was employed. The potency of a steroid in eliciting the β -glucuronidase response is defined as 24 times the reciprocal of the dose required to produce a kidney assaying 10,000 units/g. The standard of reference is testosterone. According to this measure, testosterone propionate shows a potency of 60 and that of testosterone is 3.0.

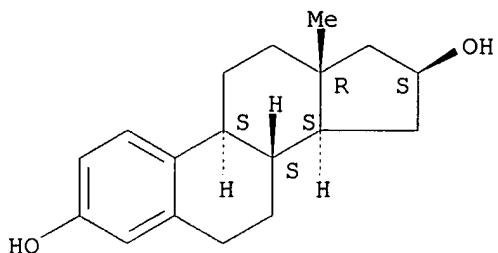
Nortestosterone cyclopentylpropionate was the most potent compd. (potency 150). There is a marked difference in response between testosterone propionate and its other esters vs. testosterone. 3,16. β -Estradiol and 16-oxoestrone gave 2- to 3-fold increases in renal β -glucuronidase. The introduction of a 17-Me or 17-Et group into nortestosterone increased its potency as detd. by the renal β -glucuronidase response.

IT 1225-58-7, Estra-1,3,5(10)(triene-3,16. β -diol
(potentiation of β -glucuronidase of kidneys by)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16. β .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 88 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1957:101244 HCPLUS

DOCUMENT NUMBER: 51:101244

ORIGINAL REFERENCE NO.: 51:18311d-g

TITLE: The effect of natural and synthetic estrogens on reticuloendothelial system function

AUTHOR(S): Heller, J. H.; Meier, R. M.; Zucker, R.; Mast, G. W.

CORPORATE SOURCE: New England Inst. for Med. Research, Ridgefield, CT

SOURCE: Endocrinology (1957), 61, 235-41

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

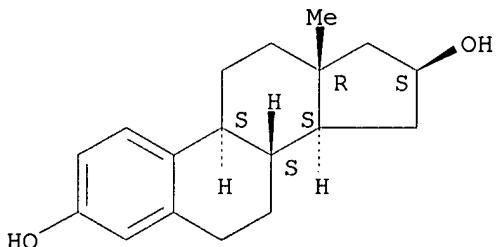
AB The activity of the reticuloendothelial system was detd. by measuring the rate of disappearance by phagocytosis of intravenously injected colloidal C from the blood. The colloid uptake of various organs was detd. by assaying for CrP32O4 content after an intravenous injection. Steroids increasing phagocytic velocity 100% or more were: estradiol, ethynylestradiol, estradiol-16-one, 1,3,5-estratriene-3,16.beta.-diol, 3-methoxy-1,3,5-estratriene-16.beta.-ol, estriol, 16-epiestriol, 3-methoxy-1,3,5-estratriene-16.beta.,17.beta.-diol, and 3-ethoxy-1,3,5-estratriene-16.beta.,17.beta.-diol; inactive were: 5-androstan-3.alpha.,16.beta.-diol, androstan-3,16.beta.-diol, androstan-3,16-dione, 5-androstan-3.beta.-ol-16-one, 4-androstan-3,16-dione, 5-androstan-3.beta.-ol-16-one, 3.beta.-methoxy-5-androstan-16-one, 1,3,5-estratriene-3,6.alpha.-diol, and 3-methoxy-1,3,5-estratriene-16-one. Stimulated activity of the reticuloendothelial system was accompanied by liver and spleen enlargement, without however, much increase in total colloid uptake by these organs.

IT 1225-58-7, Estra-1,3,5(10)(triene-3,16.beta.-diol
(effect on reticuloendothelial system)

RN 1225-58-7 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 89 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1957:47334 HCAPLUS
 DOCUMENT NUMBER: 51:47334
 ORIGINAL REFERENCE NO.: 51:8819i,8820a-h
 TITLE: 3,16.alpha.-Steroid diols
 INVENTOR(S): Huffman, Max N.
 PATENT ASSIGNEE(S): Nepera Chemical Co., Inc.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2779773		19570129	US	

AB Estrogen and androgen steroids diols with 16.alpha.-configuration and the corresponding ether and ester derivs. have considerable physiol. activity in comparison with their .beta.-isomers. 1,3,5(10)-Estratriene-3,16.beta.-diol (1 g.) in 28 ml. dry pyridine at 0.degree. treated with 4.4 g. p-MeC₆H₄SO₂Cl, the mixt. kept 2 days at room temp., dild. with ice H₂O contg. 10% NaCl, the mixt. kept 24 hrs. at 5.degree., extd. with Et₂O, and the washed and dried ext. evapd. on a steam bath gave 1.9 g. crude ditosylate, which treated with 4.8 g. freshly fused NaOEt and 92 ml. AcOH, the mixt. refluxed 1 hr. at 138-50.degree., cooled to 5.degree., treated 24 hrs. with ice H₂O contg. 10% NaCl, filtered, the dried residue saponified by refluxing 1 hr. with 200 ml. MeOH and 60 ml. 2.5N KOH, the MeOH evapd., 100 ml. H₂O added, the clear soln. treated with 10 ml. concd. HCl and the pH adjusted to 5-6 with AcOH, filtered, and the dried product (0.88 g.) recrystd. from C₆H₁₄ and aq. MeOH gave crude 3,16.alpha.-estradiol (I), m. 213-15.degree., purified through the diacetate, m. 116-17.degree., to pure I, m. 224.0-4.5.degree., [.alpha.]D₂₅ 85.degree. (c 0.76%, 95% alc.). Similarly were prep'd. 1,3,5(10),6,8-estrapentaene-3,16.alpha.-diol (II) and 1,3,5(10),7-estratetraene-3,16.alpha.-diol (III). Alkylation of II and III gave the corresponding diacetates and dipropionates. I (46 mg.) in 30 ml. 0.5N NaOH stirred with 0.5 ml. BzCl, the mixt. kept overnight at room temp., filtered, the washed residue dried in vacuo and recrystd. from Me₂CO-C₆H₁₄ and aq. MeOH gave 3-benzoxy-1,3,5(10)-estratrien-16.alpha.-ol, m. 179.5-181.0.degree.. I (150 mg.) in 6.0 ml. dry pyridine stirred 24 hrs. with 1.5 ml. BzCl, the mixt. poured into ice H₂O, the oily product crystd. from alc. Me₂CO contg. a trace of pyridine, and repeatedly recrystd. from Me₂CO-C₆H₁₄ and 95% alc. yielded 132 mg. 1,3,5(10)-estratriene-3,16.alpha.-diol dibenzoate, m. 130.5-1.5.degree.. The dipropionate, dibutyrate, divalerate, dipalmitate, distearate, bis(phenylacetate), dinaphthoate, bis(cyclopentylpropionate), and ditoluate were similarly prep'd. Treatment of 118 mg. 3-methoxy-1,3,5(10)-estratrien-16.alpha.-ol in 2 ml. pyridine with 0.2 g. p-MeC₆H₄SO₃Cl gave the corresponding 16-p-toluenesulfonate, converted by heating 1 hr. with 200 mg. fused NaOAc and 4.0 ml. AcOH to 3,16.alpha.-estradiol 3-Me ether; 16.alpha.-acetate, m. 123.0-3.5.degree.. 3.beta.-Androstanol-16-one benzoate (575 mg.) in 300 ml. MeOH was stirred 1 hr. at room temp. with 0.39 g. NaBH, the mixt. treated slowly with 4 ml. 50% AcOH, concd. to 100 ml. at 100.degree., cooled with 100 ml. ice water and the product crystd. by standing 2 days at 0.degree. to give 550 mg. 3.beta.,16.beta.-androstanediol 3-benzoate (IV), m. 168-9.degree.. IV (400 mg.) in 8 ml. dry pyridine treated with 0.8 g. p-MeC₆H₄SO₂Cl, the mixt. poured into ice water, filtered, the residue dried in vacuo, refluxed 1 hr. with 1 g.

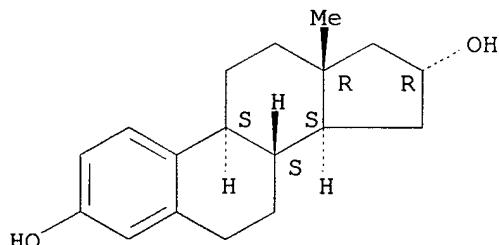
fused NaOAc and 20 ml. AcOH at 137-53.degree., the cooled mixt. extd. with Et₂O, the washed and dried ext. evapd., the residue saponified 24 hrs. in 7.5 g. KOH, 12.5 ml. H₂O, and 100 ml. MeOH, the free diol extd. with Et₂O, the washed and dried ext. evapd., and the residue purified by repeated recrystn. from Me₂CO-C₆H₁₄, MeCOEt-C₇H₁₆ and Me₂CO-C₆H₄ yielded 3.β,16.α-androstanediol (V), m. 187.5-8.0.degree., [α]_D25 -4.degree. (c 0.777, 95% alc.); diacetate, m. 174.0-4.5.degree., [α]_D23 -26.degree. (c 0.963, CHCl₃). Similarly 5-androsten-3.β-ol-one benzoate or etiocholan-3.α-ol-16-one benzoate can be transformed to the corresponding 16.β-diol and epimerized to the 16.α-diol. I (38 mg.) in 8 ml. 90% MeOH and 0.8 g. K₂CO₃ refluxed, the mixt. treated with 0.3 ml. Me₂SO₄, refluxed after the reaction with addnl. 0.3 ml. Me₂SO₄, the mixt. distd. with 4 ml. H₂O, the turbid mixt. filtered, the product washed with H₂O and dried in vacuo, taken up in Me₂CO and the soln. evapd. gave 3,16.α-estradiol 3-Me ether. Other 3-ethers are similarly prep'd. and ether groups may be formed at the 16-HO group by use of twice the amt. of dialkyl sulfates.

IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.α-diol
(effect on mammary neoplasm and phosphatases in)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.α.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L5 ANSWER 90 OF 90 HCPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1957:30854 HCPLUS

DOCUMENT NUMBER: 51:30854

ORIGINAL REFERENCE NO.: 51:5973g-i,5974a-c

TITLE: Hormonal influences on mammary tumors of the rat. I.
Acceleration of growth of transplanted fibroadenoma in
ovariectomized and hypophysectomized rats

AUTHOR(S): Huggins, Charles; Torralba, Yolanda; Mainzer, Klaus

CORPORATE SOURCE: Univ. of Chicago

SOURCE: J. Exptl. Med. (1956), 104, 525-38

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Rats were hypophysectomized (I), ovariectomized (II), or adrenalectomized (III) at 42-44 days and, at age of 51 days, were injected subcutaneously with explants of mammary fibroadenoma tissue. A variety of steroids, dissolved in EtOH and dild. with sesame oil to a 10% soln., were injected subcutaneously in 0.2 ml. doses for 6 days each week for 50 days. Protein hormones in 2% NaHCO₃ were given to some rats. At necropsy, the tumors, uteri, and inguinal mammary glands were weighed, and the content and site of alk. phosphatase detd. The tumor transplants grew in 95% of the intact

rats, by the 50th day, the increment in tumor wt. averaged 540 mg. In I rats, in II rats, and III-III rats, the tumor wts. averaged 34 mg., 182 mg. and 110 mg., resp., and the alk. phosphatase (IV) in the mammary glands averaged 0.09, 0.53, and 0.45 King-Armstrong units, resp.; glands of intact, tumor-implanted rats had an av. of 1.16 units IV. One-tenth .gamma. of estradiol-17.beta., 1.gamma. of estrone, 10-20 .gamma. of estriol, or 50 .gamma. of estradiol-3,16.alpha., injected into II rats induced optimal tumor growth, greater than that in their uninjected, intact sisters; whereas large amts., i.e., 20 .gamma., 50 .gamma., and 100 .gamma. of the 1st 3 in the above order profoundly depressed tumor growth. The mean tumor wts. in II rats receiving 19-norethynodreltestosterone, 5-androstene-3.beta.,17.beta.-diol, 4-androstene-3.alpha.,17.beta.-diol, 4-androstene-3.beta.,17.beta.-diol, 5-androsten-3.beta.-ol-17-one, and testosterone, and in intact, uninjected controls and in uninjected II rats were, resp., 750, 99, 67, 63, 57, 50, 242, and 59 mg. In II rats, estrone or estriol plus progesterone induced greater tumor wts. than did either estrogen alone. In I rats neither 1 .gamma. of estrone nor 1 mg. of progesterone, injected separately, caused an increase in tumor growth, but the two together induced considerable growth. The injection of 0.5 mg. of growth hormone, or of 1 mg. of lactogenic hormone, effected an addnl., though slight, increase in tumor wt. Small amts. of the estrogens given to II rats caused a progressive rise in the concn. of alk. phosphatase in the mammary glands.

IT 1090-04-6, Estra-1,3,5(10)-triene-3,16.alpha.-diol
(effect on mammary neoplasm and phosphatases in)

RN 1090-04-6 HCPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

